



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:48 pm BST

PDB ID : 4IOC
Title : Crystal structure of compound 4f bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Han, S.; Marr, E.S.
Deposited on : 2013-01-07
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

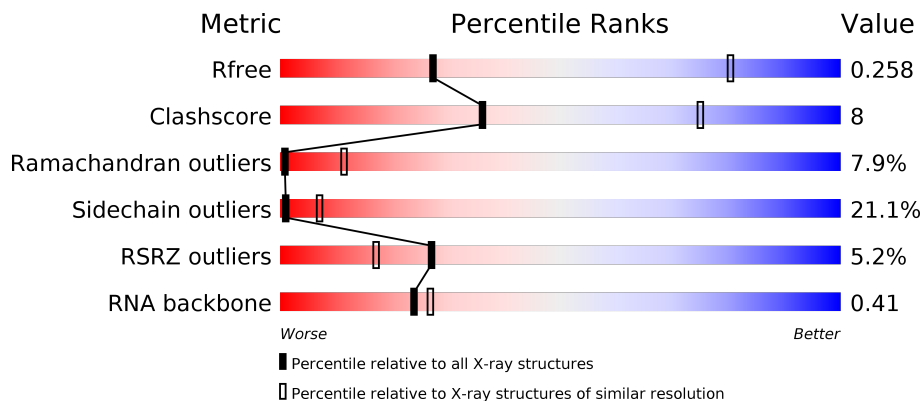
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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

Mol	Chain	Length	Quality of chain
1	X	2880	 2% 30% 38% 21% 7%
2	Y	123	 2% 27% 41% 26% 6%
3	A	274	 0% 50% 26% 11% 12%
4	B	211	 0% 62% 26% 9% 3%

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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Mol	Chain	Length	Quality of chain
30	4	37	<p>65% 70% 27%</p>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	2901	-	-	-	X
31	MG	X	2903	-	-	-	X
31	MG	X	2909	-	-	-	X
31	MG	X	2911	-	-	-	X
31	MG	X	2912	-	-	-	X
31	MG	X	2913	-	-	-	X
31	MG	X	2920	-	-	-	X
31	MG	X	2924	-	-	-	X
31	MG	X	2926	-	-	-	X
31	MG	X	2927	-	-	-	X
31	MG	X	2928	-	-	-	X
31	MG	Y	204	-	-	-	X

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 83877 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	2686	57651	25718	10642	18606	2685	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	122	2598	1161	476	840	121	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	240	1826	1137	366	321	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	205	1539	965	295	271	8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	197	1506	935	287	282	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	177	1400	892	247	254	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	E	171	1286	812	237	236	1	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	F	71	503	310	91	99	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	G	142	1114	704	209	198	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	H	134	997	614	198	180	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	I	141	1067	655	216	196		0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	J	136	1090	696	202	185	7	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	K	113	878	541	178	157	2	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	L	104	779	476	161	142	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	M	108	871	543	172	156	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	N	117	978	608	210	159	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	O	94	741	465	139	137	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	P	127	1014	639	199	174	2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	Q	93	726	458	136	130	2	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	R	110	825	513	160	151	1	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	S	175	1345	849	236	254	6	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	T	84	625	393	122	109	1	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
23	U	72	552	341	116	95	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	V	66	533	327	107	96	3	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	W	55	424	264	82	76	2	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	Z	58	457	281	94	77	5	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C 53 53	0	0	53

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

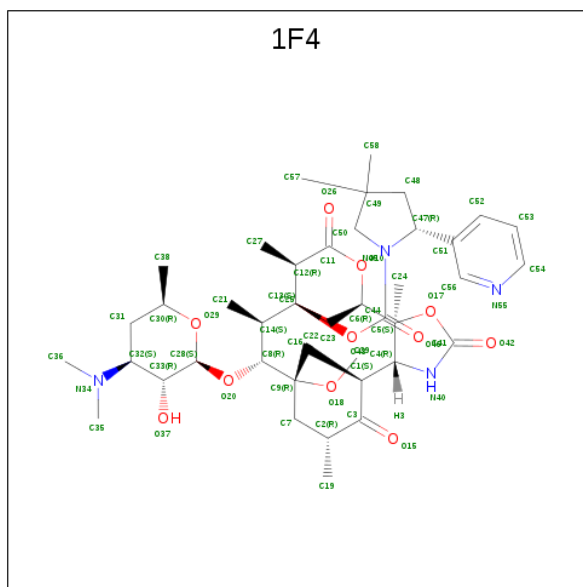
- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	28	Total Mg 28 28	0	0
31	Y	6	Total Mg 6 6	0	0
31	M	1	Total Mg 1 1	0	0

- Molecule 32 is (3aS,4R,7R,8S,9S,10R,11R,13R,15S,15aR)-4-ethyl-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,14-trioxo-10-[[3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranosyl]oxy]tetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-8-yl (2R)-4,4-dimethyl-2-(pyridin-3-yl)pyrrolidine-1-carboxylate (three-letter code: 1F4) (formula: C₄₃H₆₈N₄O₁₁).

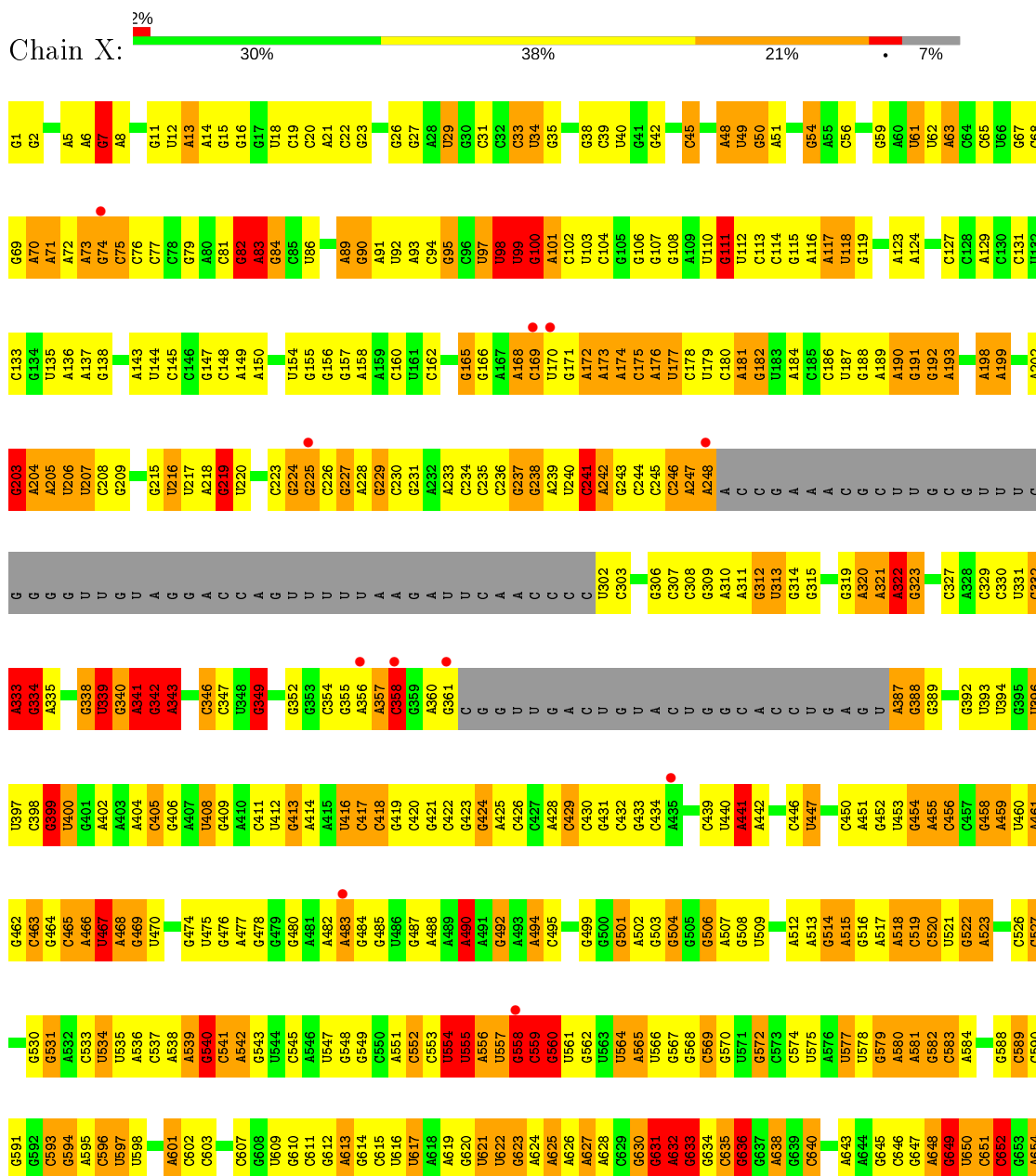


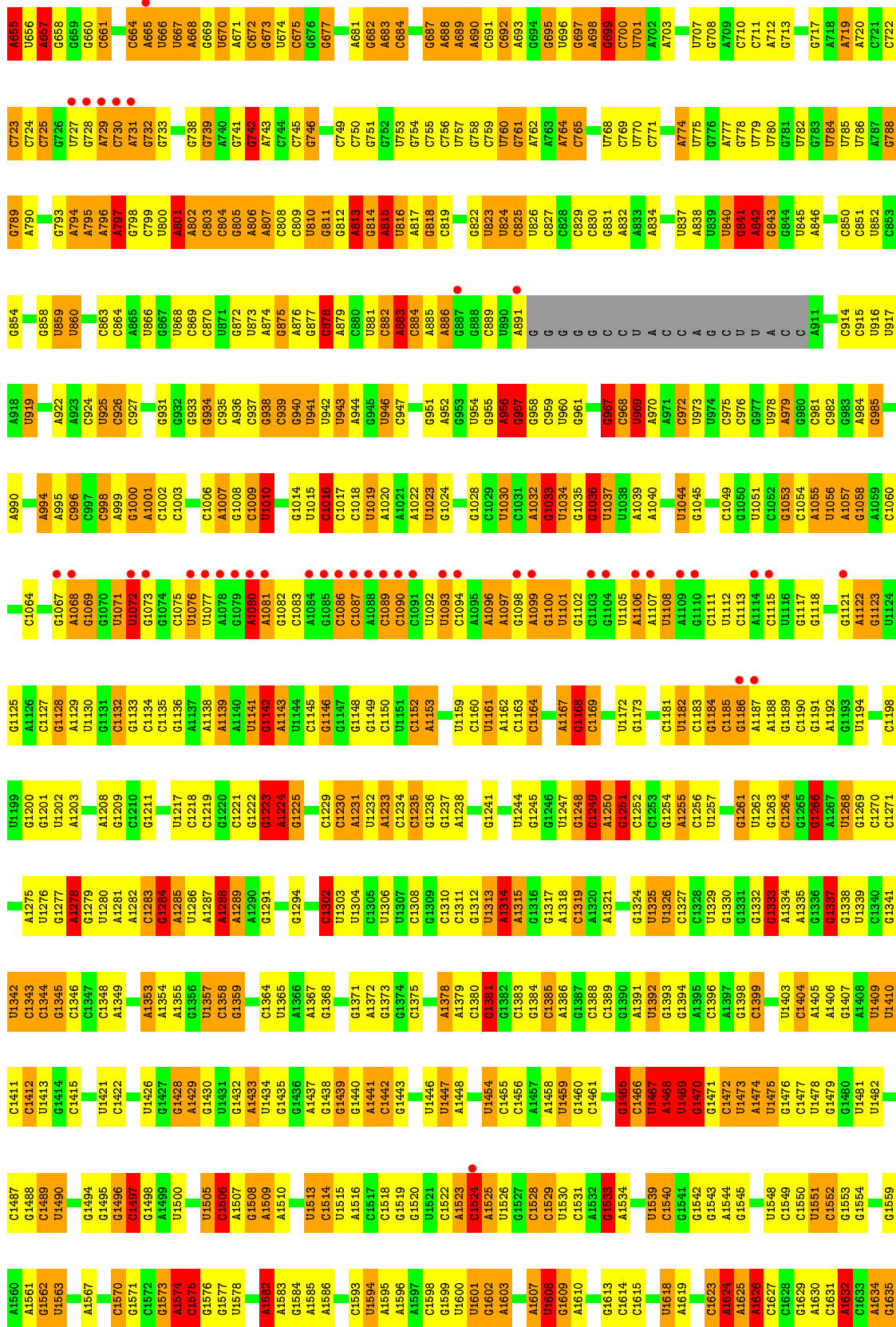
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
32	X	1	58	43	4	11	0	0

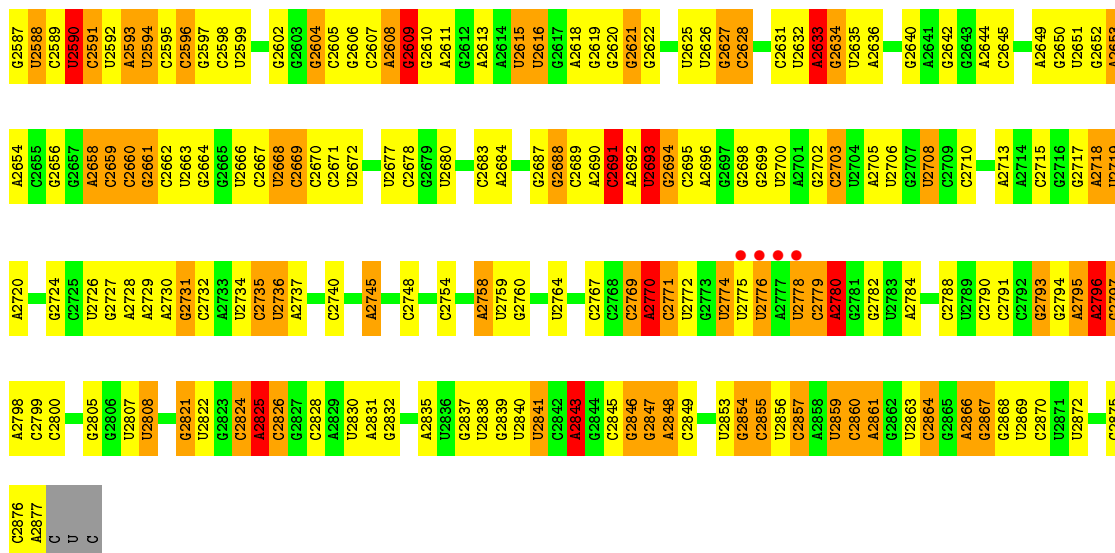
3 Residue-property plots

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

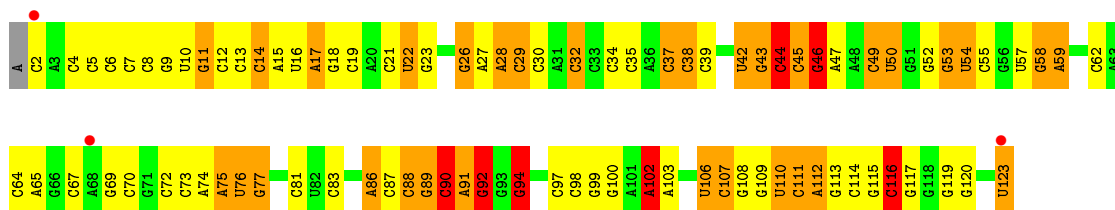
- Molecule 1: 23S ribosomal RNA



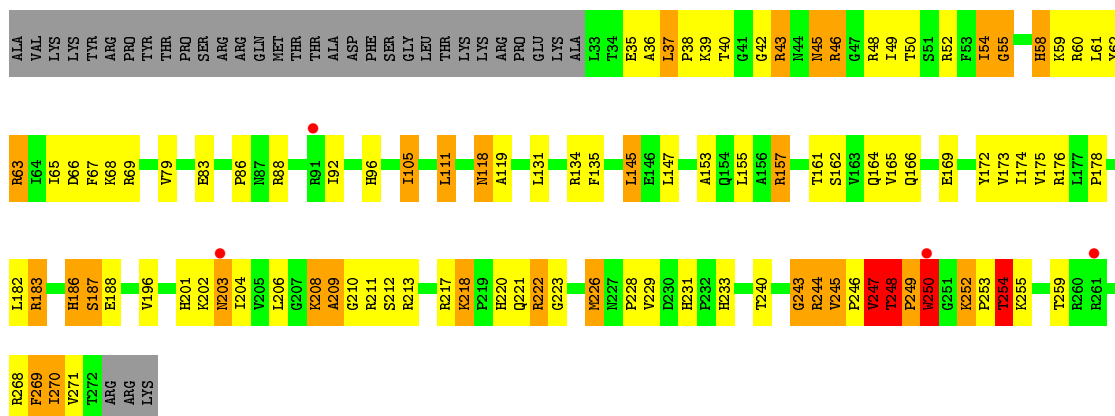




- Molecule 2: 5S ribosomal RNA

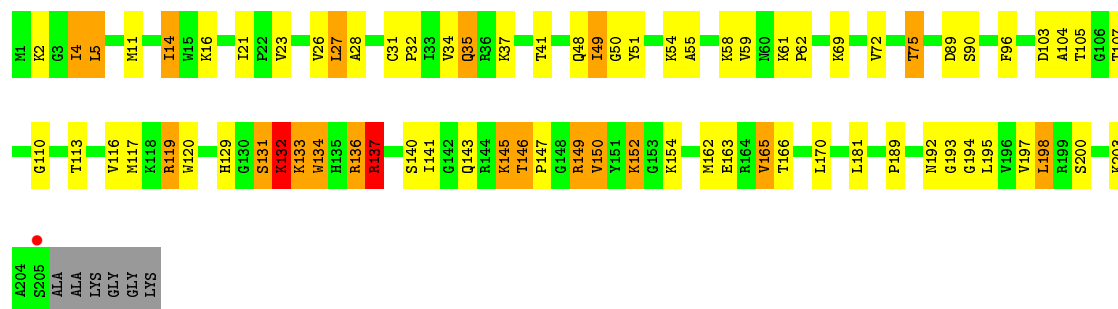


- Molecule 3: 50S ribosomal protein L2

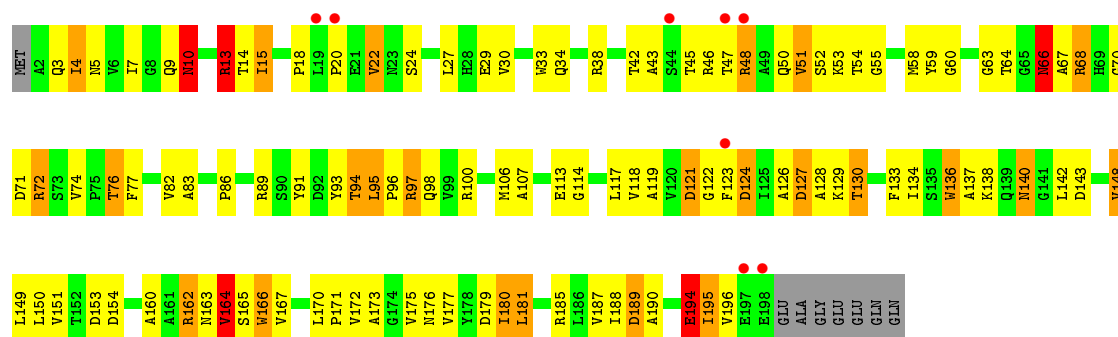
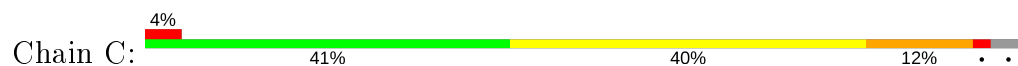


- Molecule 4: 50S ribosomal protein L3

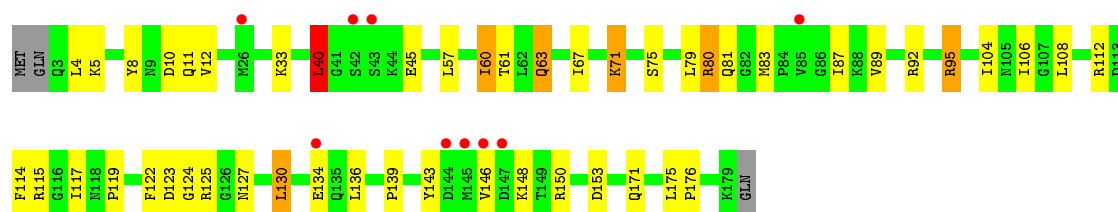




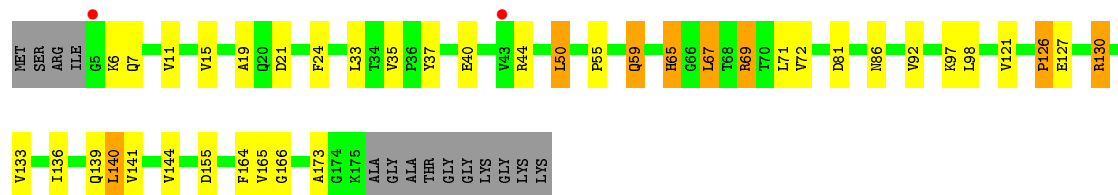
- Molecule 5: 50S ribosomal protein L4



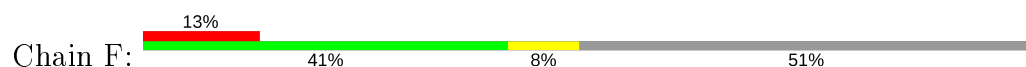
- Molecule 6: 50S ribosomal protein L5

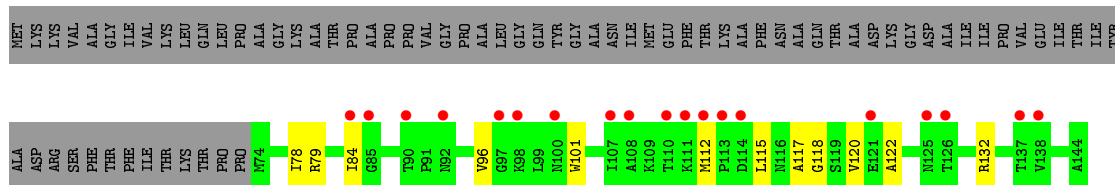


- Molecule 7: 50S ribosomal protein L6

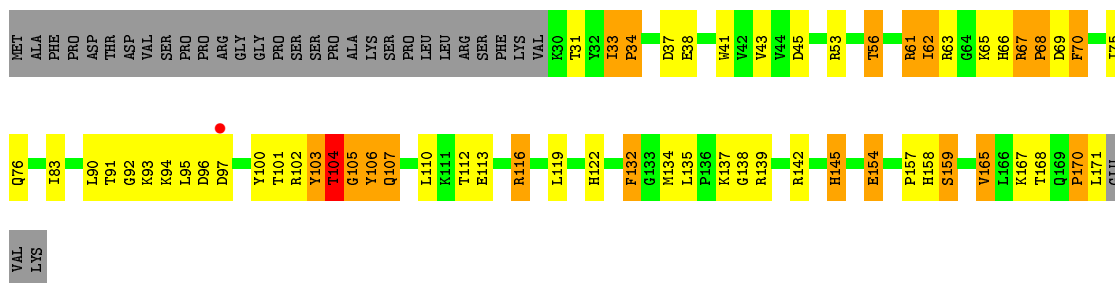


- Molecule 8: 50S ribosomal protein L11

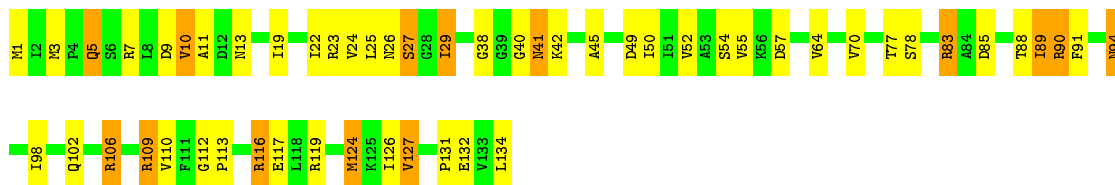




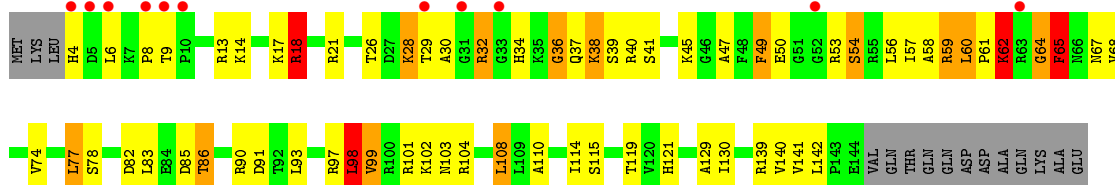
• Molecule 9: 50S ribosomal protein L13



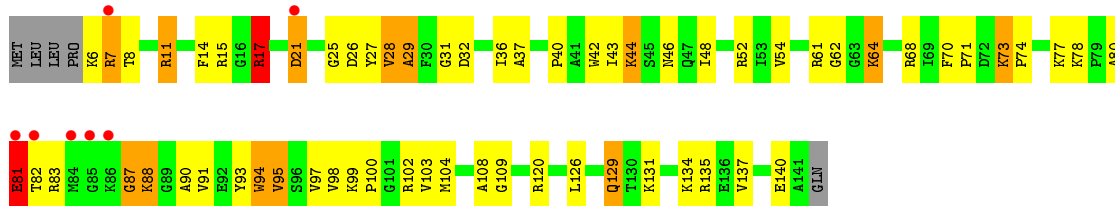
• Molecule 10: 50S ribosomal protein L14



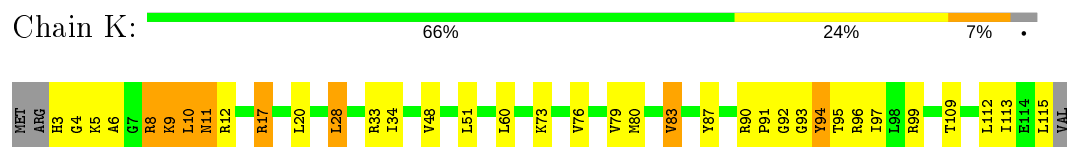
• Molecule 11: 50S ribosomal protein L15



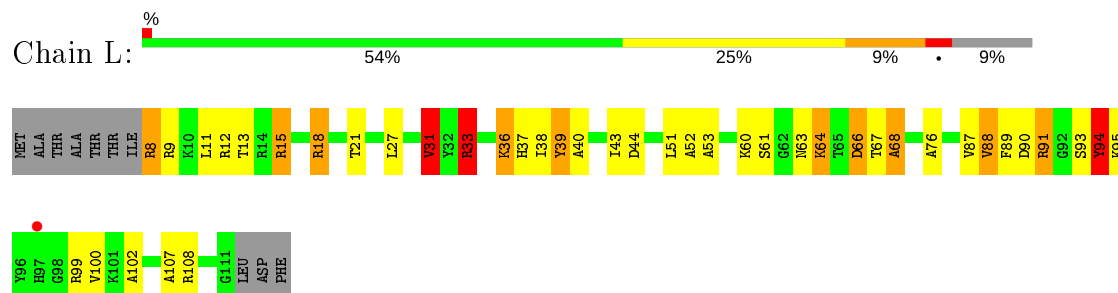
• Molecule 12: 50S ribosomal protein L16



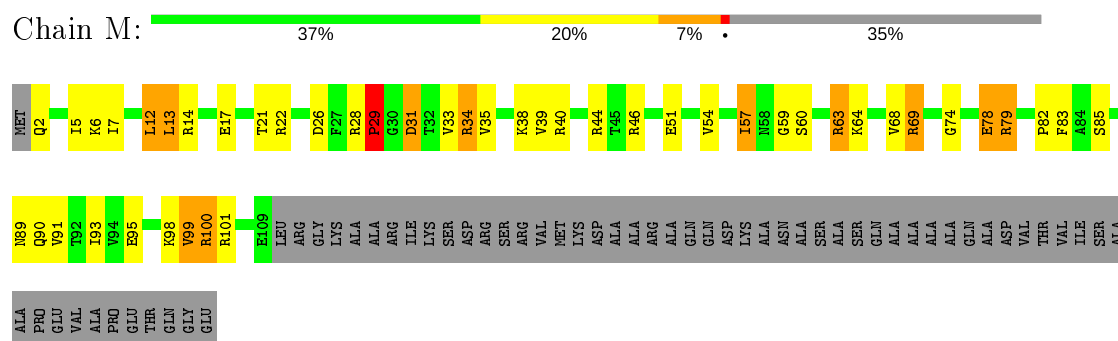
- Molecule 13: 50S ribosomal protein L17



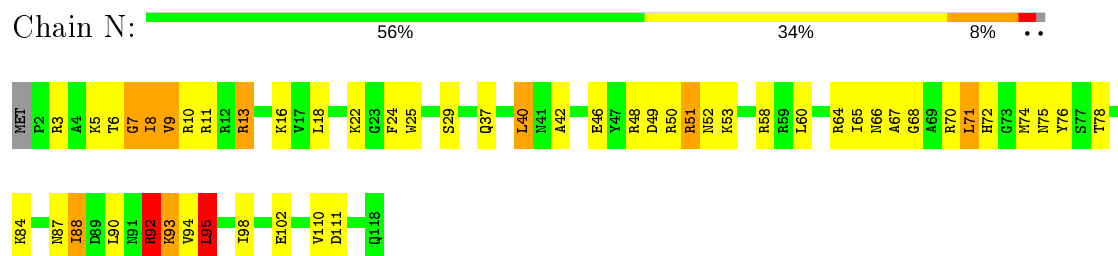
- Molecule 14: 50S ribosomal protein L18



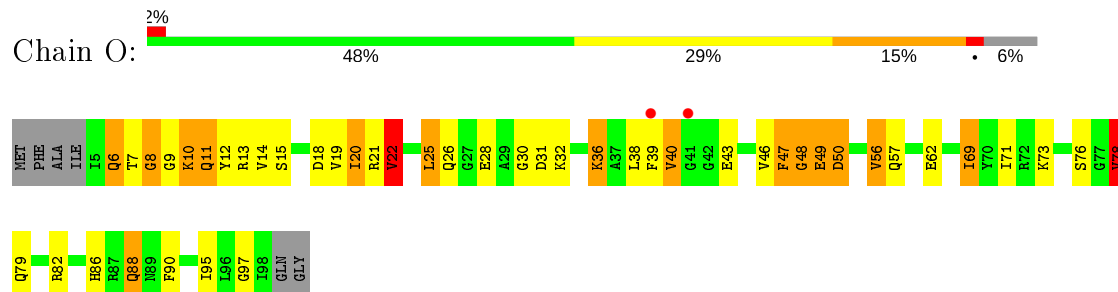
- Molecule 15: 50S ribosomal protein L19



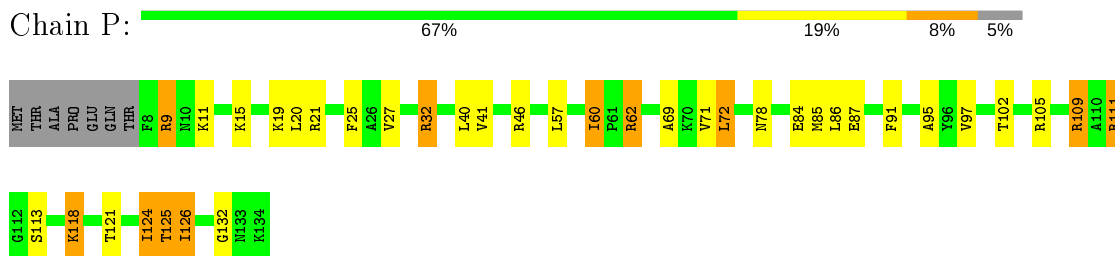
- Molecule 16: 50S ribosomal protein L20



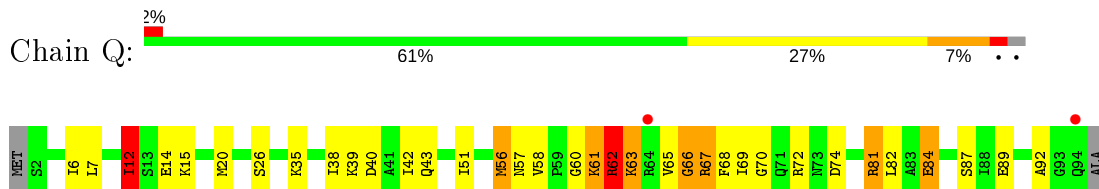
- Molecule 17: 50S ribosomal protein L21



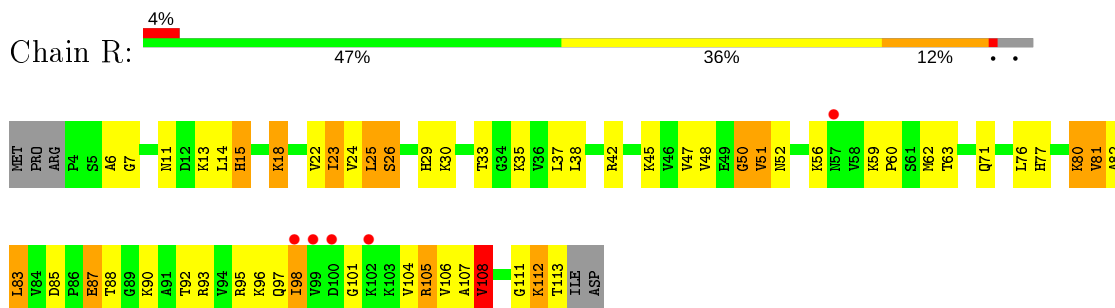
• Molecule 18: 50S ribosomal protein L22



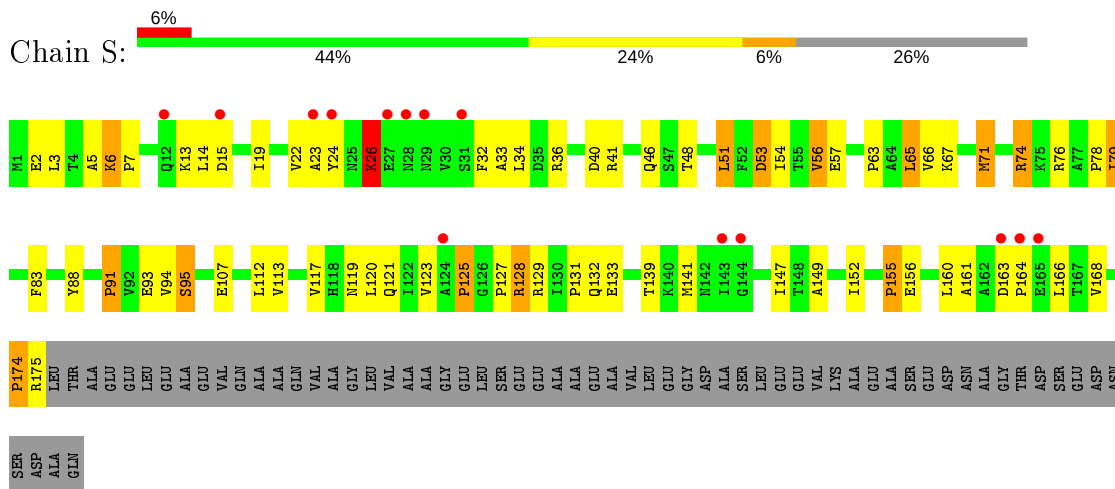
• Molecule 19: 50S ribosomal protein L23



• Molecule 20: 50S ribosomal protein L24

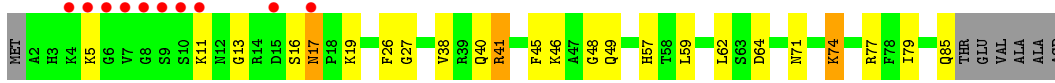


• Molecule 21: 50S ribosomal protein L25



• Molecule 22: 50S ribosomal protein L27

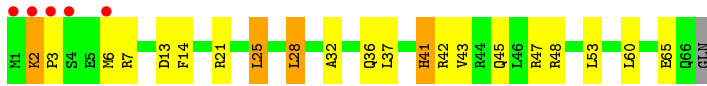




• Molecule 23: 50S ribosomal protein L28



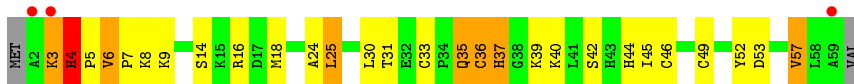
• Molecule 24: 50S ribosomal protein L29



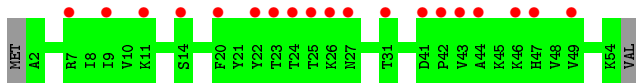
• Molecule 25: 50S ribosomal protein L30



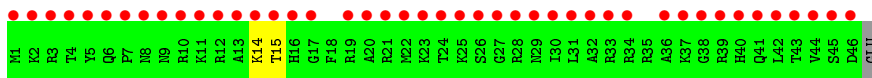
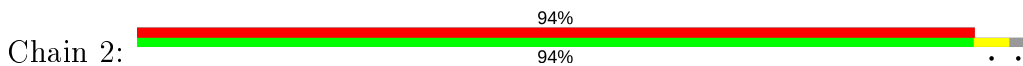
• Molecule 26: 50S ribosomal protein L32



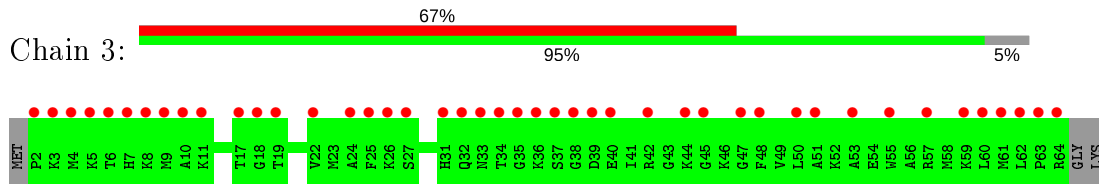
• Molecule 27: 50S ribosomal protein L33



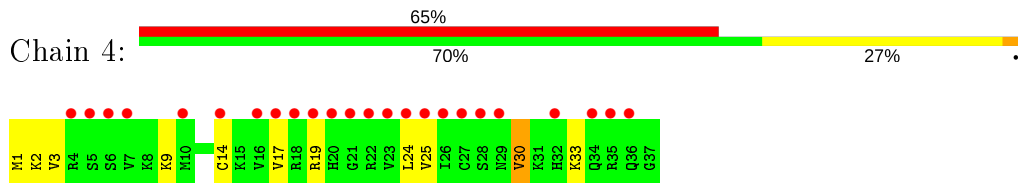
• Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.64Å 408.49Å 692.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.11 – 3.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.60) 88.4 (30.11-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.65Å)	Xtrriage
Refinement program	autobuster	Depositor
R, R_{free}	0.198 , 0.239 0.215 , 0.258	Depositor DCC
R_{free} test set	12232 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	129.2	Xtrriage
Anisotropy	0.611	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 93.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	83877	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1F4, MG

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	X	1.02	36/64561 (0.1%)	1.86	1991/100708 (2.0%)
2	Y	1.22	2/2904 (0.1%)	1.83	99/4525 (2.2%)
3	A	0.58	0/1862	0.93	4/2510 (0.2%)
4	B	0.55	0/1567	0.88	1/2105 (0.0%)
5	C	0.62	0/1529	0.96	0/2070
6	D	0.46	0/1419	0.68	0/1903
7	E	0.47	0/1308	0.71	0/1771
8	F	0.50	0/508	0.67	0/683
9	G	0.58	0/1138	0.92	2/1539 (0.1%)
10	H	0.53	0/1007	0.84	0/1352
11	I	0.67	0/1081	1.06	2/1448 (0.1%)
12	J	0.86	0/1113	0.96	1/1486 (0.1%)
13	K	0.66	0/886	0.92	0/1188
14	L	0.52	0/785	0.93	0/1048
15	M	0.59	0/884	1.00	2/1186 (0.2%)
16	N	0.53	0/994	0.79	0/1323
17	O	0.52	0/750	0.96	1/1000 (0.1%)
18	P	0.57	0/1027	0.88	0/1373
19	Q	0.56	0/737	0.99	2/988 (0.2%)
20	R	0.59	0/835	1.02	0/1121
21	S	0.61	0/1370	0.76	0/1862
22	T	0.54	0/633	0.88	0/838
23	U	0.71	0/556	1.08	2/741 (0.3%)
24	V	0.52	0/537	0.73	0/714
25	W	0.51	0/426	0.81	0/568
26	Z	0.62	0/469	0.98	0/629
30	4	0.49	0/298	0.73	0/390
All	All	0.94	38/91184 (0.0%)	1.68	2107/137069 (1.5%)

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

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	559	C	C3'-O3'	8.19	1.53	1.42
1	X	655	A	C3'-O3'	7.84	1.53	1.42
1	X	774	A	C5-C4	7.25	1.43	1.38
1	X	699	G	N9-C4	-6.97	1.32	1.38
1	X	1688	U	C2-N3	6.58	1.42	1.37
1	X	1674	C	C3'-O3'	-6.46	1.33	1.42
1	X	393	U	C1'-N1	6.43	1.58	1.48
1	X	1468	A	N7-C5	-6.24	1.35	1.39
1	X	2189	A	C3'-O3'	6.22	1.50	1.42
1	X	343	A	N9-C4	6.22	1.41	1.37
1	X	759	C	N3-C4	6.21	1.38	1.33
1	X	236	C	C1'-N1	6.10	1.57	1.48
1	X	540	G	C2-N3	5.99	1.37	1.32
1	X	346	C	C1'-N1	5.97	1.57	1.48
1	X	774	A	C6-N1	5.88	1.39	1.35
1	X	646	C	C1'-N1	5.79	1.57	1.48
1	X	2018	G	C3'-O3'	5.78	1.50	1.42
1	X	927	C	C1'-N1	5.72	1.57	1.48
1	X	868	U	C1'-N1	5.65	1.57	1.48
1	X	917	U	C1'-N1	5.60	1.57	1.48
1	X	1522	C	C1'-N1	5.52	1.57	1.48
1	X	1946	U	C1'-N1	5.45	1.56	1.48
2	Y	87	C	C3'-O3'	5.44	1.49	1.42
1	X	774	A	N3-C4	5.37	1.38	1.34
1	X	434	C	C1'-N1	5.35	1.56	1.48
1	X	31	C	C1'-N1	5.30	1.56	1.48
2	Y	32	C	C1'-N1	5.27	1.56	1.48
1	X	1688	U	N3-C4	5.25	1.43	1.38
1	X	422	C	C1'-N1	5.18	1.56	1.48
1	X	327	C	C1'-N1	5.15	1.56	1.48
1	X	2072	C	C1'-N1	5.14	1.56	1.48
1	X	1182	U	C1'-N1	5.14	1.56	1.48
1	X	2321	C	C1'-N1	5.14	1.56	1.48
1	X	1825	C	C1'-N1	5.11	1.56	1.48
1	X	358	C	C1'-N1	5.08	1.56	1.48
1	X	558	G	C3'-O3'	5.08	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	430	C	C1'-N1	5.06	1.56	1.48
1	X	774	A	N1-C2	5.03	1.38	1.34

All (2107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-30.77	85.29	109.90
1	X	1019	U	P-O3'-C3'	19.01	142.51	119.70
1	X	1288	A	C5'-C4'-O4'	18.79	131.64	109.10
1	X	774	A	N1-C6-N6	17.73	129.24	118.60
1	X	559	C	O4'-C1'-N1	17.43	122.14	108.20
1	X	2808	U	O4'-C1'-N1	16.51	121.41	108.20
1	X	1288	A	O4'-C1'-N9	16.46	121.37	108.20
1	X	2564	U	P-O3'-C3'	16.04	138.95	119.70
1	X	176	A	P-O3'-C3'	15.97	138.86	119.70
1	X	655	A	P-O3'-C3'	15.78	138.64	119.70
1	X	558	G	P-O3'-C3'	15.40	138.18	119.70
1	X	1775	A	P-O3'-C3'	15.14	137.87	119.70
1	X	1278	A	O4'-C1'-N9	14.65	119.92	108.20
1	X	1473	U	P-O3'-C3'	14.53	137.13	119.70
1	X	204	A	P-O3'-C3'	14.46	137.05	119.70
1	X	33	C	P-O3'-C3'	14.32	136.88	119.70
1	X	1634	A	P-O3'-C3'	14.15	136.69	119.70
1	X	100	G	P-O3'-C3'	14.14	136.66	119.70
1	X	559	C	C4'-C3'-C2'	-14.06	88.54	102.60
1	X	2497	A	P-O3'-C3'	13.90	136.38	119.70
1	X	2736	U	P-O3'-C3'	13.74	136.19	119.70
1	X	2018	G	P-O3'-C3'	13.71	136.16	119.70
1	X	814	G	P-O3'-C3'	13.68	136.11	119.70
1	X	1790	G	P-O3'-C3'	13.67	136.11	119.70
1	X	342	G	P-O3'-C3'	13.52	135.92	119.70
1	X	2312	A	P-O3'-C3'	13.31	135.68	119.70
1	X	994	A	P-O3'-C3'	13.30	135.66	119.70
1	X	774	A	N7-C8-N9	13.21	120.41	113.80
1	X	334	G	P-O3'-C3'	13.15	135.48	119.70
1	X	788	G	P-O3'-C3'	13.06	135.38	119.70
1	X	1475	U	P-O3'-C3'	12.98	135.28	119.70
1	X	181	A	P-O3'-C3'	12.91	135.19	119.70
1	X	1574	A	O4'-C1'-N9	12.86	118.49	108.20
1	X	343	A	O4'-C1'-N9	12.82	118.46	108.20
1	X	664	C	P-O3'-C3'	12.82	135.08	119.70
1	X	1468	A	C8-N9-C4	-12.70	100.72	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	48	A	P-O3'-C3'	12.66	134.89	119.70
1	X	683	A	P-O3'-C3'	12.61	134.82	119.70
1	X	1036	G	P-O3'-C3'	12.58	134.79	119.70
1	X	1938	U	P-O3'-C3'	12.51	134.71	119.70
1	X	469	G	P-O3'-C3'	12.51	134.71	119.70
1	X	2323	U	P-O3'-C3'	12.48	134.68	119.70
1	X	774	A	C5-N7-C8	-12.45	97.68	103.90
1	X	559	C	P-O3'-C3'	12.37	134.54	119.70
1	X	2854	G	C1'-O4'-C4'	-12.31	100.05	109.90
1	X	774	A	C6-C5-N7	-12.29	123.70	132.30
1	X	2691	C	P-O3'-C3'	12.27	134.42	119.70
1	X	399	G	P-O3'-C3'	12.25	134.40	119.70
1	X	1249	G	P-O3'-C3'	12.20	134.34	119.70
1	X	822	G	P-O3'-C3'	12.20	134.34	119.70
1	X	2261	G	P-O3'-C3'	12.06	134.17	119.70
1	X	537	C	N1-C2-O2	11.88	126.03	118.90
1	X	218	A	P-O3'-C3'	11.84	133.91	119.70
1	X	73	A	P-O3'-C3'	11.83	133.90	119.70
1	X	1442	C	P-O3'-C3'	11.82	133.88	119.70
1	X	33	C	O4'-C1'-N1	11.81	117.65	108.20
1	X	454	G	P-O3'-C3'	11.81	133.87	119.70
1	X	514	G	P-O3'-C3'	11.70	133.74	119.70
1	X	1441	A	P-O3'-C3'	11.69	133.72	119.70
2	Y	58	G	P-O3'-C3'	11.69	133.72	119.70
1	X	2854	G	N9-C1'-C2'	11.57	129.04	114.00
1	X	540	G	N1-C6-O6	-11.44	113.04	119.90
1	X	2298	U	P-O3'-C3'	11.43	133.41	119.70
1	X	774	A	C4-C5-N7	11.39	116.39	110.70
1	X	2189	A	P-O3'-C3'	11.34	133.30	119.70
1	X	98	U	P-O3'-C3'	11.30	133.26	119.70
1	X	1096	A	P-O3'-C3'	11.30	133.26	119.70
1	X	490	A	P-O3'-C3'	11.30	133.26	119.70
1	X	1391	A	P-O3'-C3'	11.28	133.24	119.70
1	X	2426	G	P-O3'-C3'	11.26	133.21	119.70
1	X	1122	A	P-O3'-C3'	11.22	133.16	119.70
1	X	1288	A	C4'-C3'-C2'	-11.03	91.57	102.60
2	Y	16	U	P-O3'-C3'	11.01	132.91	119.70
1	X	841	G	O4'-C4'-C3'	-11.00	93.00	104.00
1	X	1746	A	O4'-C1'-N9	10.89	116.91	108.20
1	X	1923	U	P-O3'-C3'	10.88	132.76	119.70
1	X	554	U	P-O3'-C3'	10.87	132.74	119.70
1	X	522	G	O4'-C1'-N9	10.80	116.84	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	691	C	O4'-C1'-N1	10.80	116.84	108.20
1	X	1468	A	O4'-C1'-C2'	-10.79	95.00	105.80
1	X	1261	G	P-O3'-C3'	10.78	132.64	119.70
1	X	699	G	N3-C4-N9	-10.76	119.54	126.00
1	X	2491	C	O4'-C1'-N1	10.75	116.80	108.20
1	X	71	A	P-O3'-C3'	10.72	132.57	119.70
1	X	2770	A	P-O3'-C3'	10.71	132.55	119.70
1	X	1186	G	P-O3'-C3'	10.64	132.47	119.70
1	X	2371	A	O4'-C1'-N9	10.63	116.71	108.20
1	X	242	A	C1'-O4'-C4'	-10.63	101.40	109.90
1	X	1632	A	O4'-C1'-N9	-10.53	99.78	108.20
1	X	333	A	P-O3'-C3'	10.48	132.27	119.70
1	X	2634	G	O4'-C1'-N9	10.44	116.55	108.20
1	X	1820	G	P-O3'-C3'	10.44	132.22	119.70
1	X	1732	U	P-O3'-C3'	10.42	132.21	119.70
1	X	1053	G	P-O3'-C3'	10.38	132.16	119.70
1	X	1333	G	N3-C4-N9	-10.31	119.81	126.00
1	X	1280	U	P-O3'-C3'	10.29	132.04	119.70
1	X	699	G	N3-C4-C5	10.28	133.74	128.60
1	X	1055	A	P-O3'-C3'	10.26	132.01	119.70
1	X	805	G	O4'-C1'-N9	-10.22	100.02	108.20
1	X	809	C	O4'-C1'-N1	10.21	116.37	108.20
1	X	1684	G	P-O3'-C3'	10.16	131.90	119.70
1	X	2731	G	P-O3'-C3'	10.16	131.89	119.70
1	X	1403	U	P-O3'-C3'	10.15	131.88	119.70
1	X	1409	U	P-O3'-C3'	10.14	131.87	119.70
1	X	341	A	P-O3'-C3'	10.14	131.87	119.70
1	X	2593	A	P-O3'-C3'	10.11	131.83	119.70
1	X	321	A	P-O3'-C3'	10.11	131.83	119.70
1	X	1474	A	P-O3'-C3'	10.10	131.82	119.70
1	X	2018	G	C1'-O4'-C4'	-10.01	101.89	109.90
1	X	434	C	P-O3'-C3'	9.91	131.60	119.70
1	X	666	U	O4'-C1'-N1	9.91	116.13	108.20
1	X	89	A	P-O3'-C3'	9.91	131.59	119.70
1	X	813	A	P-O3'-C3'	9.89	131.57	119.70
1	X	651	C	P-O3'-C3'	9.83	131.50	119.70
1	X	2228	U	P-O3'-C3'	9.83	131.50	119.70
1	X	1278	A	C1'-O4'-C4'	-9.83	102.03	109.90
1	X	655	A	O4'-C1'-N9	9.83	116.06	108.20
1	X	1799	A	C1'-O4'-C4'	-9.77	102.09	109.90
1	X	2229	G	P-O3'-C3'	9.77	131.42	119.70
1	X	540	G	P-O3'-C3'	9.76	131.41	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	467	U	P-O3'-C3'	9.73	131.38	119.70
1	X	2730	A	P-O3'-C3'	9.73	131.37	119.70
1	X	1601	U	P-O3'-C3'	9.68	131.32	119.70
1	X	1770	U	C1'-O4'-C4'	-9.68	102.16	109.90
1	X	1086	C	P-O3'-C3'	9.66	131.29	119.70
1	X	1976	U	O4'-C1'-N1	9.66	115.92	108.20
1	X	1353	A	P-O3'-C3'	9.65	131.28	119.70
1	X	2689	C	P-O3'-C3'	9.58	131.20	119.70
1	X	638	A	P-O3'-C3'	9.57	131.19	119.70
1	X	1975	G	P-O3'-C3'	9.56	131.17	119.70
1	X	632	A	O4'-C1'-N9	9.53	115.83	108.20
1	X	343	A	C8-N9-C4	-9.53	101.99	105.80
1	X	2330	G	N9-C1'-C2'	9.53	126.38	114.00
1	X	731	A	P-O3'-C3'	9.52	131.12	119.70
1	X	483	A	P-O3'-C3'	-9.50	108.30	119.70
1	X	1278	A	C3'-C2'-C1'	-9.50	93.90	101.50
1	X	1811	A	P-O3'-C3'	9.49	131.09	119.70
1	X	172	A	P-O3'-C3'	9.48	131.08	119.70
1	X	242	A	O4'-C1'-N9	9.46	115.77	108.20
1	X	557	U	C1'-O4'-C4'	-9.45	102.34	109.90
1	X	803	C	P-O3'-C3'	9.45	131.04	119.70
1	X	939	C	P-O3'-C3'	9.43	131.01	119.70
1	X	1575	C	P-O3'-C3'	9.43	131.01	119.70
1	X	1489	C	O4'-C1'-N1	9.39	115.71	108.20
1	X	646	C	O4'-C1'-N1	9.36	115.69	108.20
1	X	2190	A	O4'-C1'-N9	9.36	115.69	108.20
1	X	2591	C	N1-C2-O2	9.34	124.50	118.90
1	X	1574	A	C1'-O4'-C4'	-9.32	102.44	109.90
2	Y	90	C	P-O3'-C3'	-9.30	108.53	119.70
1	X	1313	U	O4'-C1'-N1	9.29	115.64	108.20
1	X	1459	U	P-O3'-C3'	9.29	130.85	119.70
1	X	1338	G	P-O3'-C3'	9.28	130.84	119.70
1	X	34	U	O4'-C1'-N1	9.27	115.62	108.20
1	X	841	G	O4'-C1'-N9	9.25	115.60	108.20
1	X	1439	G	P-O3'-C3'	9.23	130.78	119.70
1	X	941	U	O4'-C1'-N1	9.21	115.57	108.20
1	X	2222	U	O4'-C1'-N1	9.21	115.57	108.20
1	X	2324	G	P-O3'-C3'	9.17	130.71	119.70
1	X	2566	A	P-O3'-C3'	9.13	130.65	119.70
1	X	1663	C	N1-C2-O2	9.12	124.37	118.90
1	X	2634	G	C3'-C2'-C1'	-9.12	94.21	101.50
1	X	2039	G	C8-N9-C4	-9.11	102.75	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	247	A	C1'-O4'-C4'	-9.11	102.61	109.90
2	Y	81	C	O4'-C1'-N1	9.11	115.48	108.20
1	X	2472	U	P-O3'-C3'	-9.09	108.79	119.70
1	X	494	A	P-O3'-C3'	9.08	130.60	119.70
1	X	883	A	C5'-C4'-O4'	9.07	119.99	109.10
1	X	1790	G	O4'-C1'-N9	9.05	115.44	108.20
1	X	416	U	O4'-C1'-N1	9.01	115.41	108.20
1	X	2270	U	O4'-C1'-N1	9.01	115.41	108.20
1	X	312	G	C1'-O4'-C4'	-8.99	102.71	109.90
1	X	841	G	N9-C1'-C2'	8.97	125.66	114.00
1	X	656	U	P-O3'-C3'	8.95	130.44	119.70
1	X	1333	G	C8-N9-C4	-8.95	102.82	106.40
1	X	1984	A	C3'-C2'-C1'	-8.95	94.34	101.50
1	X	2018	G	C5-N7-C8	-8.95	99.83	104.30
1	X	2626	U	O4'-C1'-N1	8.95	115.36	108.20
1	X	1688	U	N3-C4-O4	8.93	125.65	119.40
1	X	817	A	C1'-O4'-C4'	-8.91	102.77	109.90
1	X	774	A	C5-C6-N1	-8.91	113.25	117.70
1	X	2018	G	C4-C5-N7	8.91	114.36	110.80
1	X	332	C	O4'-C1'-N1	8.84	115.27	108.20
1	X	755	C	P-O3'-C3'	-8.82	109.11	119.70
1	X	1268	U	P-O3'-C3'	8.77	130.22	119.70
1	X	825	C	P-O3'-C3'	-8.73	109.22	119.70
1	X	938	G	P-O3'-C3'	8.73	130.18	119.70
1	X	774	A	N9-C4-C5	-8.73	102.31	105.80
1	X	2228	U	N3-C4-C5	-8.73	109.36	114.60
1	X	976	C	O4'-C1'-N1	8.73	115.18	108.20
1	X	666	U	C1'-O4'-C4'	-8.71	102.94	109.90
1	X	845	U	O4'-C1'-N1	8.70	115.16	108.20
1	X	320	A	O4'-C1'-N9	8.68	115.15	108.20
1	X	2034	A	P-O3'-C3'	8.68	130.12	119.70
1	X	1496	G	P-O3'-C3'	8.67	130.11	119.70
1	X	173	A	C1'-O4'-C4'	-8.67	102.97	109.90
1	X	1574	A	C4'-C3'-C2'	-8.67	93.93	102.60
1	X	1790	G	C1'-O4'-C4'	-8.64	102.99	109.90
1	X	2204	A	P-O3'-C3'	8.60	130.02	119.70
1	X	1288	A	C3'-C2'-C1'	-8.60	94.62	101.50
1	X	99	U	P-O3'-C3'	8.58	130.00	119.70
1	X	1161	U	O4'-C1'-N1	8.58	115.06	108.20
1	X	817	A	O4'-C4'-C3'	-8.57	95.43	104.00
1	X	2824	C	P-O3'-C3'	8.57	129.98	119.70
1	X	2039	G	N9-C4-C5	8.56	108.83	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1710	U	P-O3'-C3'	8.56	129.97	119.70
1	X	236	C	O4'-C1'-N1	8.56	115.05	108.20
1	X	1468	A	O4'-C1'-N9	8.55	115.04	108.20
1	X	841	G	C8-N9-C4	-8.54	102.99	106.40
1	X	358	C	O4'-C1'-N1	8.53	115.02	108.20
2	Y	86	A	O4'-C1'-N9	8.49	115.00	108.20
1	X	2414	A	P-O3'-C3'	8.49	129.89	119.70
1	X	2051	U	O4'-C1'-N1	8.47	114.98	108.20
1	X	1072	U	P-O3'-C3'	8.46	129.85	119.70
1	X	761	G	C1'-O4'-C4'	-8.45	103.14	109.90
1	X	216	U	O4'-C1'-N1	8.45	114.96	108.20
1	X	432	C	O4'-C1'-N1	8.44	114.95	108.20
1	X	2452	U	P-O3'-C3'	8.44	129.83	119.70
1	X	2481	G	P-O3'-C3'	8.44	129.82	119.70
1	X	2497	A	C1'-O4'-C4'	-8.43	103.15	109.90
1	X	1468	A	P-O3'-C3'	8.43	129.82	119.70
1	X	346	C	N1-C1'-C2'	8.43	124.96	114.00
1	X	2018	G	N9-C1'-C2'	8.43	124.96	114.00
1	X	774	A	C5-C6-N6	-8.42	116.96	123.70
1	X	577	U	O4'-C1'-N1	8.41	114.93	108.20
1	X	2703	C	O4'-C1'-N1	8.41	114.93	108.20
1	X	515	A	P-O3'-C3'	8.41	129.79	119.70
1	X	117	A	P-O3'-C3'	8.40	129.78	119.70
1	X	577	U	C4'-C3'-C2'	-8.39	94.21	102.60
1	X	1333	G	O4'-C1'-N9	8.39	114.91	108.20
1	X	1705	U	O4'-C1'-N1	8.39	114.91	108.20
1	X	2025	A	O4'-C1'-N9	8.39	114.91	108.20
1	X	1466	C	C6-N1-C2	-8.36	116.96	120.30
1	X	1966	C	O4'-C1'-N1	8.34	114.88	108.20
1	X	518	A	P-O3'-C3'	8.34	129.70	119.70
1	X	1731	C	O4'-C1'-N1	8.33	114.86	108.20
2	Y	88	C	O4'-C1'-N1	8.32	114.85	108.20
1	X	2853	U	O4'-C1'-N1	8.31	114.85	108.20
1	X	1467	U	N1-C2-O2	8.30	128.61	122.80
1	X	940	G	P-O5'-C5'	8.29	134.17	120.90
1	X	1524	C	P-O3'-C3'	8.29	129.65	119.70
1	X	2196	U	P-O3'-C3'	8.29	129.64	119.70
1	X	579	G	C4-C5-N7	-8.28	107.49	110.80
1	X	2439	U	O4'-C1'-N1	8.28	114.82	108.20
1	X	387	A	C5'-C4'-O4'	8.27	119.03	109.10
1	X	2370	G	O4'-C1'-N9	8.26	114.81	108.20
1	X	2228	U	N3-C4-O4	8.26	125.18	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2778	U	P-O3'-C3'	8.26	129.61	119.70
1	X	2237	C	P-O3'-C3'	8.24	129.59	119.70
1	X	2198	U	P-O3'-C3'	8.23	129.58	119.70
1	X	582	G	P-O3'-C3'	8.22	129.57	119.70
1	X	2669	C	N1-C2-O2	8.21	123.83	118.90
1	X	184	A	O4'-C1'-N9	8.21	114.77	108.20
1	X	192	G	P-O3'-C3'	8.19	129.53	119.70
1	X	190	A	O4'-C1'-N9	8.19	114.75	108.20
1	X	650	U	O4'-C1'-N1	8.19	114.75	108.20
1	X	1223	G	C3'-C2'-C1'	8.19	108.05	101.50
1	X	2859	U	O4'-C1'-N1	8.19	114.75	108.20
1	X	1975	G	C2'-C3'-O3'	8.18	127.50	109.50
1	X	1917	C	O4'-C1'-N1	8.17	114.73	108.20
1	X	2409	A	C1'-O4'-C4'	-8.16	103.38	109.90
1	X	394	U	O4'-C1'-N1	8.15	114.72	108.20
1	X	1468	A	C3'-C2'-C1'	-8.14	94.99	101.50
1	X	1468	A	N7-C8-N9	8.13	117.87	113.80
1	X	1991	C	P-O3'-C3'	-8.13	109.94	119.70
1	X	969	U	P-O3'-C3'	8.13	129.45	119.70
1	X	2291	U	O4'-C1'-N1	8.13	114.70	108.20
1	X	1467	U	N1-C1'-C2'	8.12	124.56	114.00
1	X	1285	A	P-O3'-C3'	8.11	129.43	119.70
1	X	1315	A	P-O3'-C3'	8.10	129.42	119.70
1	X	2795	A	P-O3'-C3'	8.10	129.42	119.70
1	X	338	G	C8-N9-C4	-8.09	103.16	106.40
1	X	2758	A	C1'-O4'-C4'	-8.08	103.43	109.90
1	X	1749	G	C1'-O4'-C4'	-8.08	103.43	109.90
1	X	2726	U	O4'-C1'-N1	8.05	114.64	108.20
2	Y	90	C	O4'-C1'-N1	8.05	114.64	108.20
1	X	1313	U	C1'-O4'-C4'	-8.05	103.46	109.90
1	X	841	G	C1'-O4'-C4'	-8.02	103.48	109.90
1	X	1412	C	P-O3'-C3'	8.02	129.32	119.70
1	X	843	G	P-O3'-C3'	8.02	129.32	119.70
1	X	2531	U	N3-C2-O2	-7.99	116.61	122.20
1	X	2693	U	C1'-O4'-C4'	-7.99	103.51	109.90
1	X	2258	G	C4'-C3'-C2'	-7.98	94.62	102.60
1	X	2432	A	O4'-C1'-N9	7.97	114.58	108.20
1	X	1345	G	C5'-C4'-O4'	7.97	118.66	109.10
1	X	242	A	C4'-C3'-C2'	-7.96	94.64	102.60
1	X	1656	U	P-O3'-C3'	7.95	129.24	119.70
1	X	1288	A	O4'-C4'-C3'	-7.95	96.05	104.00
1	X	499	G	O4'-C1'-N9	7.94	114.55	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1523	A	P-O3'-C3'	7.93	129.22	119.70
1	X	1217	U	O4'-C1'-N1	7.92	114.54	108.20
2	Y	54	U	O4'-C1'-N1	7.92	114.53	108.20
1	X	1850	G	P-O3'-C3'	7.90	129.18	119.70
1	X	938	G	O4'-C1'-N9	7.89	114.51	108.20
1	X	458	G	P-O3'-C3'	7.87	129.14	119.70
1	X	346	C	C6-N1-C2	-7.87	117.15	120.30
1	X	882	C	O4'-C1'-N1	7.87	114.49	108.20
1	X	1188	A	P-O3'-C3'	7.85	129.12	119.70
1	X	509	U	O4'-C1'-N1	7.85	114.48	108.20
1	X	1339	U	P-O3'-C3'	7.84	129.11	119.70
1	X	2507	U	P-O3'-C3'	7.84	129.11	119.70
1	X	1830	C	P-O3'-C3'	7.84	129.10	119.70
1	X	1467	U	P-O3'-C3'	-7.83	110.30	119.70
1	X	1469	U	N3-C2-O2	-7.82	116.72	122.20
1	X	1152	C	P-O3'-C3'	7.82	129.08	119.70
1	X	593	C	O4'-C1'-N1	7.80	114.44	108.20
1	X	2702	G	C5-C6-O6	-7.78	123.93	128.60
1	X	2049	C	O4'-C1'-N1	7.76	114.41	108.20
1	X	696	U	O4'-C1'-N1	7.76	114.41	108.20
1	X	2485	U	O4'-C1'-N1	-7.75	102.00	108.20
1	X	1791	C	O4'-C1'-N1	7.74	114.39	108.20
1	X	816	U	O4'-C1'-N1	7.74	114.39	108.20
1	X	2872	U	O4'-C1'-N1	7.73	114.38	108.20
1	X	2860	C	O4'-C1'-N1	7.73	114.38	108.20
1	X	1496	G	C3'-C2'-C1'	-7.71	95.33	101.50
1	X	223	C	O4'-C1'-N1	7.71	114.36	108.20
1	X	1777	A	C1'-O4'-C4'	-7.71	103.73	109.90
1	X	2664	G	N1-C6-O6	7.70	124.52	119.90
1	X	357	A	P-O3'-C3'	7.69	128.93	119.70
1	X	1172	U	O4'-C1'-N1	7.69	114.36	108.20
1	X	2651	U	O4'-C1'-N1	7.68	114.35	108.20
1	X	2788	C	O4'-C1'-N1	7.68	114.34	108.20
1	X	2288	A	P-O3'-C3'	7.68	128.91	119.70
1	X	2039	G	O4'-C1'-N9	7.68	114.34	108.20
1	X	868	U	O4'-C1'-N1	7.67	114.34	108.20
1	X	1268	U	O4'-C1'-N1	7.67	114.34	108.20
1	X	2481	G	C5-C6-O6	-7.67	124.00	128.60
1	X	2018	G	C3'-C2'-C1'	-7.66	95.37	101.50
1	X	2530	C	P-O3'-C3'	7.66	128.90	119.70
1	X	2664	G	C6-C5-N7	-7.66	125.80	130.40
1	X	198	A	P-O3'-C3'	7.66	128.89	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	742	G	P-O3'-C3'	7.66	128.89	119.70
1	X	1071	U	P-O3'-C3'	7.66	128.89	119.70
1	X	1618	U	P-O3'-C3'	7.65	128.88	119.70
1	X	2274	C	O4'-C1'-N1	7.65	114.32	108.20
1	X	18	U	O4'-C1'-N1	7.65	114.32	108.20
1	X	308	C	O4'-C1'-N1	7.63	114.30	108.20
1	X	690	A	C4'-C3'-C2'	-7.63	94.97	102.60
1	X	788	G	C1'-O4'-C4'	-7.61	103.81	109.90
1	X	636	G	C8-N9-C4	-7.61	103.36	106.40
1	X	1302	C	O4'-C1'-N1	7.59	114.28	108.20
1	X	1935	A	N9-C1'-C2'	7.59	123.87	114.00
1	X	2005	U	O4'-C1'-N1	7.58	114.27	108.20
1	X	926	C	O4'-C1'-N1	7.58	114.27	108.20
1	X	1654	A	C3'-C2'-C1'	-7.58	95.44	101.50
1	X	774	A	P-O5'-C5'	7.56	133.00	120.90
1	X	937	C	O4'-C1'-N1	7.55	114.24	108.20
1	X	2841	U	O4'-C1'-N1	7.55	114.24	108.20
1	X	1327	C	C5-C6-N1	7.54	124.77	121.00
1	X	1001	A	P-O3'-C3'	7.54	128.75	119.70
1	X	2671	C	O4'-C1'-N1	7.54	114.23	108.20
1	X	2460	G	P-O5'-C5'	7.54	132.97	120.90
1	X	2460	G	O4'-C1'-N9	7.53	114.23	108.20
1	X	2190	A	C1'-O4'-C4'	-7.53	103.88	109.90
1	X	247	A	O4'-C1'-N9	7.52	114.22	108.20
1	X	1211	G	P-O3'-C3'	-7.52	110.68	119.70
1	X	242	A	P-O3'-C3'	7.51	128.71	119.70
2	Y	29	C	O4'-C1'-N1	7.51	114.21	108.20
1	X	1357	U	P-O3'-C3'	7.51	128.71	119.70
1	X	1433	A	O4'-C1'-N9	7.51	114.20	108.20
1	X	307	C	O4'-C1'-N1	7.50	114.20	108.20
1	X	2015	G	P-O3'-C3'	7.49	128.69	119.70
1	X	925	U	P-O3'-C3'	7.49	128.69	119.70
1	X	2431	C	O4'-C1'-N1	7.49	114.19	108.20
1	X	626	A	P-O3'-C3'	7.48	128.68	119.70
1	X	2694	G	P-O3'-C3'	7.48	128.68	119.70
2	Y	30	C	O4'-C1'-N1	7.48	114.18	108.20
1	X	1283	C	P-O3'-C3'	7.47	128.67	119.70
1	X	2710	C	O4'-C1'-N1	7.47	114.17	108.20
1	X	1221	C	O4'-C1'-N1	7.47	114.17	108.20
1	X	1223	G	P-O3'-C3'	7.47	128.66	119.70
1	X	2056	C	P-O3'-C3'	7.46	128.66	119.70
1	X	2477	C	P-O5'-C5'	7.46	132.84	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1985	G	O4'-C1'-N9	7.46	114.17	108.20
1	X	2384	G	P-O3'-C3'	7.46	128.65	119.70
1	X	94	C	O4'-C1'-N1	7.46	114.17	108.20
2	Y	26	G	P-O3'-C3'	7.45	128.64	119.70
1	X	2830	U	O4'-C1'-N1	7.45	114.16	108.20
1	X	2660	C	O4'-C1'-N1	7.44	114.15	108.20
1	X	2088	U	P-O3'-C3'	7.44	128.63	119.70
1	X	837	U	O4'-C1'-N1	7.44	114.15	108.20
1	X	177	U	O4'-C1'-N1	7.43	114.14	108.20
1	X	1664	G	O5'-P-OP2	7.43	119.61	110.70
1	X	2580	C	P-O3'-C3'	7.43	128.61	119.70
1	X	841	G	N7-C8-N9	7.42	116.81	113.10
1	X	117	A	O4'-C1'-N9	7.41	114.13	108.20
1	X	1607	A	P-O3'-C3'	7.41	128.59	119.70
1	X	2033	C	P-O3'-C3'	7.40	128.58	119.70
1	X	2799	C	O4'-C1'-N1	7.40	114.12	108.20
1	X	1681	A	P-O3'-C3'	7.40	128.58	119.70
1	X	2633	A	P-O3'-C3'	7.40	128.58	119.70
1	X	2564	U	C1'-O4'-C4'	-7.40	103.98	109.90
1	X	1412	C	O4'-C1'-N1	7.39	114.12	108.20
1	X	1142	G	P-O3'-C3'	7.39	128.57	119.70
1	X	2258	G	O4'-C1'-N9	7.39	114.11	108.20
1	X	1469	U	P-O5'-C5'	7.38	132.70	120.90
1	X	1412	C	C3'-C2'-C1'	-7.36	95.61	101.50
1	X	2662	C	C4'-C3'-C2'	-7.36	95.24	102.60
1	X	1559	G	P-O3'-C3'	7.35	128.52	119.70
1	X	31	C	O4'-C1'-N1	7.34	114.07	108.20
1	X	788	G	N9-C1'-C2'	7.34	123.54	114.00
1	X	796	A	C4'-C3'-C2'	-7.33	95.27	102.60
1	X	1909	U	O4'-C1'-N1	7.33	114.06	108.20
1	X	815	A	P-O3'-C3'	7.33	128.49	119.70
1	X	1688	U	N3-C4-C5	-7.32	110.21	114.60
1	X	92	U	O4'-C1'-N1	7.32	114.06	108.20
1	X	2298	U	O4'-C1'-N1	7.31	114.05	108.20
1	X	1143	A	C5'-C4'-O4'	7.30	117.86	109.10
1	X	1051	U	O4'-C1'-N1	7.30	114.04	108.20
1	X	2006	G	O4'-C1'-N9	7.30	114.04	108.20
1	X	1000	G	O4'-C1'-N9	7.29	114.03	108.20
1	X	2239	C	O4'-C1'-N1	7.29	114.03	108.20
1	X	2290	A	P-O3'-C3'	7.28	128.44	119.70
1	X	567	G	O4'-C1'-N9	7.28	114.02	108.20
1	X	742	G	C1'-O4'-C4'	-7.28	104.08	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	539	A	C1'-O4'-C4'	-7.27	104.09	109.90
1	X	1439	G	C3'-C2'-C1'	-7.27	95.69	101.50
1	X	180	C	O4'-C1'-N1	7.26	114.01	108.20
1	X	2702	G	N1-C6-O6	7.24	124.25	119.90
1	X	972	C	C1'-O4'-C4'	-7.24	104.11	109.90
1	X	2561	G	C5-C6-O6	-7.24	124.26	128.60
1	X	1333	G	N9-C4-C5	7.24	108.30	105.40
1	X	2870	C	O4'-C1'-N1	7.23	113.99	108.20
1	X	875	G	O4'-C1'-N9	7.23	113.99	108.20
1	X	2267	A	P-O3'-C3'	7.23	128.38	119.70
1	X	2560	G	C8-N9-C4	-7.23	103.51	106.40
1	X	2634	G	C1'-O4'-C4'	-7.23	104.12	109.90
1	X	564	U	O4'-C1'-N1	7.23	113.98	108.20
1	X	1776	A	P-O3'-C3'	7.23	128.37	119.70
1	X	1865	C	O4'-C1'-N1	7.23	113.98	108.20
1	X	1080	A	C1'-O4'-C4'	-7.22	104.12	109.90
1	X	1920	A	P-O3'-C3'	7.22	128.37	119.70
1	X	520	C	P-O3'-C3'	7.22	128.36	119.70
1	X	1513	U	O4'-C1'-N1	7.22	113.97	108.20
1	X	61	U	C1'-O4'-C4'	-7.21	104.13	109.90
1	X	631	G	O4'-C1'-N9	7.21	113.97	108.20
1	X	2608	A	C1'-O4'-C4'	-7.21	104.13	109.90
2	Y	19	C	N1-C2-O2	7.21	123.22	118.90
1	X	174	A	P-O3'-C3'	7.20	128.34	119.70
1	X	430	C	O4'-C1'-N1	7.20	113.96	108.20
1	X	802	A	O4'-C1'-N9	-7.19	102.45	108.20
1	X	1467	U	C4-C5-C6	-7.19	115.39	119.70
2	Y	106	U	O4'-C1'-N1	7.19	113.95	108.20
1	X	465	C	P-O5'-C5'	-7.19	109.40	120.90
1	X	810	U	P-O3'-C3'	-7.19	111.08	119.70
1	X	1289	A	O4'-C1'-N9	-7.18	102.45	108.20
1	X	1461	C	O4'-C1'-N1	7.18	113.95	108.20
1	X	1218	C	O4'-C1'-N1	7.18	113.94	108.20
1	X	1310	C	O4'-C1'-N1	7.18	113.94	108.20
1	X	331	U	O4'-C1'-N1	7.17	113.94	108.20
1	X	2284	U	O4'-C1'-N1	7.17	113.93	108.20
1	X	81	C	O4'-C1'-N1	7.16	113.93	108.20
1	X	531	G	P-O3'-C3'	-7.16	111.11	119.70
1	X	518	A	N9-C1'-C2'	7.15	123.29	114.00
1	X	2509	A	P-O3'-C3'	7.13	128.26	119.70
1	X	2026	C	N3-C2-O2	-7.13	116.91	121.90
1	X	117	A	C1'-O4'-C4'	-7.13	104.20	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2039	G	N3-C2-N2	-7.12	114.91	119.90
1	X	2449	G	O4'-C1'-N9	7.12	113.90	108.20
1	X	758	G	O4'-C1'-N9	7.12	113.90	108.20
1	X	514	G	N9-C1'-C2'	7.12	123.25	114.00
1	X	526	C	C3'-C2'-C1'	-7.11	95.81	101.50
1	X	1788	C	O4'-C1'-N1	7.11	113.89	108.20
1	X	943	U	O4'-C1'-N1	7.11	113.88	108.20
1	X	1938	U	N1-C1'-C2'	7.11	123.24	114.00
1	X	2338	C	P-O3'-C3'	7.11	128.23	119.70
1	X	455	A	P-O3'-C3'	7.10	128.22	119.70
1	X	2705	A	P-O3'-C3'	7.10	128.22	119.70
1	X	59	G	P-O3'-C3'	7.10	128.22	119.70
1	X	1652	G	P-O3'-C3'	7.09	128.21	119.70
2	Y	92	G	P-O3'-C3'	-7.09	111.19	119.70
1	X	1364	C	O4'-C1'-N1	7.09	113.87	108.20
1	X	2620	G	C4'-C3'-C2'	-7.09	95.51	102.60
2	Y	6	C	O4'-C1'-N1	7.08	113.87	108.20
1	X	2691	C	O4'-C1'-N1	7.07	113.86	108.20
1	X	2699	G	P-O3'-C3'	7.07	128.18	119.70
1	X	2243	C	O4'-C1'-N1	7.07	113.85	108.20
1	X	1950	C	O4'-C1'-N1	7.06	113.85	108.20
1	X	2498	U	P-O3'-C3'	7.06	128.17	119.70
1	X	558	G	N9-C1'-C2'	7.05	123.17	114.00
1	X	343	A	N7-C8-N9	7.04	117.32	113.80
1	X	1772	C	O4'-C1'-N1	7.04	113.84	108.20
1	X	1966	C	P-O3'-C3'	-7.04	111.25	119.70
1	X	2403	C	N1-C2-O2	7.04	123.13	118.90
1	X	2567	G	C8-N9-C4	-7.04	103.58	106.40
1	X	822	G	C4'-C3'-C2'	-7.04	95.56	102.60
1	X	1975	G	O4'-C1'-N9	-7.04	102.57	108.20
1	X	2782	G	O4'-C1'-N9	7.04	113.83	108.20
1	X	1723	U	O4'-C1'-N1	7.03	113.82	108.20
1	X	1470	G	P-O5'-C5'	-7.03	109.66	120.90
1	X	2845	C	O4'-C1'-N1	7.03	113.82	108.20
1	X	1201	G	P-O3'-C3'	7.02	128.13	119.70
1	X	2238	G	O4'-C1'-N9	7.02	113.82	108.20
1	X	190	A	C1'-O4'-C4'	-7.02	104.28	109.90
1	X	756	C	N1-C2-O2	7.02	123.11	118.90
1	X	2795	A	C3'-C2'-C1'	7.02	107.11	101.50
1	X	2593	A	O3'-P-O5'	-7.00	90.69	104.00
1	X	2080	U	O4'-C1'-N1	7.00	113.80	108.20
1	X	1403	U	O4'-C1'-N1	7.00	113.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	801	A	P-O3'-C3'	6.99	128.09	119.70
1	X	1754	G	P-O3'-C3'	6.99	128.08	119.70
1	X	113	C	O4'-C1'-N1	6.98	113.79	108.20
1	X	2550	C	O4'-C1'-N1	6.97	113.78	108.20
1	X	1711	C	C1'-O4'-C4'	-6.97	104.32	109.90
1	X	2406	C	P-O3'-C3'	6.96	128.06	119.70
1	X	399	G	C4'-C3'-C2'	6.96	109.56	102.60
1	X	946	U	O4'-C1'-N1	6.95	113.76	108.20
1	X	2662	C	N1-C2-O2	6.95	123.07	118.90
1	X	1458	A	P-O3'-C3'	6.94	128.03	119.70
1	X	796	A	N1-C6-N6	6.94	122.76	118.60
1	X	74	G	O4'-C4'-C3'	-6.93	97.07	104.00
1	X	2072	C	O4'-C1'-N1	6.93	113.74	108.20
1	X	814	G	N9-C1'-C2'	6.93	123.01	114.00
1	X	1308	C	C3'-C2'-C1'	-6.92	95.96	101.50
1	X	2551	A	P-O3'-C3'	6.92	128.01	119.70
1	X	1801	C	P-O3'-C3'	6.92	128.01	119.70
1	X	2782	G	C1'-O4'-C4'	-6.92	104.36	109.90
1	X	1139	A	N9-C1'-C2'	6.92	122.99	114.00
1	X	2794	G	P-O3'-C3'	6.91	127.99	119.70
2	Y	107	C	P-O3'-C3'	6.91	127.99	119.70
1	X	2488	G	P-O3'-C3'	-6.90	111.42	119.70
1	X	83	A	C1'-O4'-C4'	-6.90	104.38	109.90
1	X	95	G	P-O3'-C3'	6.90	127.98	119.70
1	X	1409	U	C1'-O4'-C4'	-6.90	104.38	109.90
1	X	2667	C	N1-C2-O2	6.90	123.04	118.90
1	X	1108	U	O4'-C1'-N1	6.89	113.71	108.20
1	X	2030	U	P-O3'-C3'	-6.89	111.43	119.70
1	X	560	G	P-O3'-C3'	-6.89	111.44	119.70
1	X	2533	U	O4'-C1'-N1	6.88	113.71	108.20
1	X	1313	U	C3'-C2'-C1'	-6.88	96.00	101.50
1	X	483	A	N9-C1'-C2'	6.88	122.94	114.00
1	X	826	U	O4'-C1'-N1	6.88	113.70	108.20
1	X	636	G	N7-C8-N9	6.87	116.54	113.10
2	Y	32	C	C6-N1-C2	-6.87	117.55	120.30
1	X	247	A	P-O3'-C3'	6.87	127.94	119.70
2	Y	74	A	P-O3'-C3'	6.87	127.94	119.70
1	X	2217	G	C1'-O4'-C4'	-6.87	104.41	109.90
1	X	796	A	C5-N7-C8	-6.87	100.47	103.90
1	X	1487	C	O4'-C1'-N1	6.87	113.69	108.20
1	X	2691	C	C1'-O4'-C4'	-6.86	104.41	109.90
1	X	1422	C	O4'-C1'-N1	6.86	113.69	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2018	G	O4'-C1'-C2'	-6.85	98.95	105.80
1	X	774	A	C8-N9-C4	-6.85	103.06	105.80
1	X	1086	C	O4'-C1'-N1	6.85	113.68	108.20
1	X	1522	C	C3'-C2'-C1'	-6.85	96.02	101.50
1	X	1602	G	P-O3'-C3'	6.84	127.91	119.70
1	X	2418	A	P-O3'-C3'	6.84	127.91	119.70
1	X	1200	G	O4'-C1'-N9	6.83	113.67	108.20
1	X	1465	G	P-O3'-C3'	-6.83	111.50	119.70
1	X	927	C	C6-N1-C2	-6.83	117.57	120.30
1	X	2245	A	P-O3'-C3'	6.82	127.89	119.70
1	X	617	U	N3-C2-O2	-6.82	117.42	122.20
2	Y	90	C	C3'-C2'-C1'	-6.82	96.05	101.50
1	X	1433	A	C1'-O4'-C4'	-6.82	104.45	109.90
2	Y	37	C	O4'-C1'-N1	6.81	113.65	108.20
1	X	1469	U	P-O3'-C3'	6.81	127.88	119.70
1	X	1963	G	P-O3'-C3'	6.81	127.87	119.70
1	X	527	C	C5-C6-N1	6.81	124.41	121.00
1	X	170	U	N3-C2-O2	-6.81	117.43	122.20
1	X	567	G	P-O3'-C3'	-6.81	111.53	119.70
1	X	1410	U	O4'-C1'-N1	6.80	113.64	108.20
1	X	580	A	N9-C1'-C2'	6.80	122.83	114.00
1	X	1686	A	C1'-O4'-C4'	-6.80	104.46	109.90
1	X	1466	C	N3-C2-O2	-6.79	117.14	121.90
1	X	1656	U	O4'-C1'-N1	6.79	113.64	108.20
1	X	1745	C	O4'-C1'-N1	6.79	113.63	108.20
1	X	2339	A	O4'-C1'-N9	6.79	113.63	108.20
2	Y	123	U	C2-N1-C1'	6.79	125.85	117.70
1	X	2554	C	O4'-C1'-N1	6.78	113.63	108.20
1	X	699	G	O4'-C1'-N9	6.78	113.62	108.20
1	X	1164	C	O4'-C1'-N1	6.78	113.62	108.20
1	X	39	C	O4'-C1'-N1	6.78	113.62	108.20
2	Y	44	C	O4'-C1'-N1	6.77	113.62	108.20
1	X	542	A	C5-N7-C8	-6.77	100.52	103.90
1	X	514	G	O4'-C1'-N9	-6.76	102.79	108.20
1	X	559	C	C5'-C4'-O4'	6.76	117.22	109.10
1	X	582	G	N3-C4-C5	-6.76	125.22	128.60
2	Y	17	A	P-O3'-C3'	6.75	127.80	119.70
1	X	1526	U	O4'-C1'-N1	6.75	113.60	108.20
1	X	2672	U	N1-C2-O2	6.75	127.52	122.80
1	X	477	A	O5'-P-OP2	-6.74	99.63	105.70
1	X	1652	G	C6-C5-N7	-6.74	126.36	130.40
1	X	886	A	C3'-C2'-C1'	-6.74	96.11	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2347	C	O4'-C1'-N1	6.74	113.59	108.20
1	X	2590	U	P-O5'-C5'	6.73	131.67	120.90
1	X	1608	U	O4'-C1'-N1	6.73	113.58	108.20
1	X	2479	U	C5-C6-N1	6.73	126.06	122.70
1	X	2579	A	C3'-C2'-C1'	6.72	106.88	101.50
1	X	870	C	O4'-C1'-N1	6.72	113.58	108.20
1	X	2855	C	P-O3'-C3'	-6.72	111.64	119.70
1	X	2022	C	O4'-C1'-N1	6.72	113.57	108.20
1	X	501	G	O4'-C1'-N9	6.71	113.57	108.20
1	X	697	G	O4'-C1'-N9	6.71	113.57	108.20
1	X	1958	G	O4'-C4'-C3'	-6.71	97.29	104.00
1	X	575	U	P-O3'-C3'	6.71	127.75	119.70
2	Y	53	G	N3-C4-C5	-6.71	125.25	128.60
1	X	739	G	O4'-C1'-N9	6.70	113.56	108.20
1	X	1632	A	P-O3'-C3'	6.70	127.75	119.70
1	X	1792	C	P-O3'-C3'	6.70	127.75	119.70
1	X	1833	U	O4'-C1'-N1	6.70	113.56	108.20
1	X	1184	G	P-O3'-C3'	6.70	127.74	119.70
1	X	208	C	O4'-C1'-N1	6.70	113.56	108.20
1	X	1308	C	P-O5'-C5'	-6.69	110.19	120.90
1	X	133	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	699	G	P-O3'-C3'	6.69	127.73	119.70
1	X	1163	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	2838	U	O4'-C1'-N1	6.69	113.55	108.20
2	Y	8	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	1468	A	N9-C1'-C2'	6.69	122.70	114.00
1	X	2392	G	O4'-C1'-N9	6.69	113.55	108.20
1	X	864	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	1663	C	P-O3'-C3'	6.69	127.73	119.70
1	X	1743	C	P-O3'-C3'	-6.69	111.67	119.70
1	X	1979	C	P-O3'-C3'	6.69	127.73	119.70
1	X	624	A	O4'-C1'-N9	6.69	113.55	108.20
1	X	823	U	O4'-C1'-N1	6.69	113.55	108.20
2	Y	87	C	O4'-C1'-N1	6.68	113.55	108.20
1	X	2538	C	N1-C2-O2	6.68	122.91	118.90
1	X	1744	G	C4'-C3'-C2'	-6.68	95.92	102.60
1	X	234	C	N1-C2-O2	6.68	122.91	118.90
1	X	2483	U	O4'-C1'-N1	6.67	113.54	108.20
1	X	2574	G	O4'-C1'-N9	6.67	113.54	108.20
1	X	2256	G	C8-N9-C4	-6.67	103.73	106.40
1	X	2190	A	P-O3'-C3'	6.66	127.70	119.70
1	X	83	A	P-O3'-C3'	6.66	127.69	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1068	A	P-O3'-C3'	6.66	127.69	119.70
1	X	2459	C	N1-C2-O2	6.66	122.90	118.90
1	X	649	G	O4'-C1'-N9	6.66	113.53	108.20
1	X	1404	C	O4'-C1'-N1	6.66	113.53	108.20
1	X	2854	G	P-O3'-C3'	6.66	127.69	119.70
1	X	1343	C	O4'-C1'-N1	6.65	113.52	108.20
1	X	559	C	C1'-O4'-C4'	-6.64	104.58	109.90
1	X	1232	U	O4'-C1'-N1	6.64	113.52	108.20
1	X	1927	U	P-O3'-C3'	6.64	127.67	119.70
1	X	346	C	C2-N1-C1'	6.64	126.11	118.80
1	X	1716	G	O3'-P-O5'	-6.64	91.38	104.00
1	X	559	C	C3'-C2'-C1'	6.64	106.81	101.50
1	X	996	C	N1-C2-O2	6.64	122.88	118.90
1	X	2487	G	O4'-C1'-N9	6.64	113.51	108.20
1	X	689	A	C1'-O4'-C4'	-6.63	104.59	109.90
1	X	343	A	O4'-C1'-C2'	-6.63	99.17	105.80
1	X	578	U	O4'-C1'-N1	6.63	113.51	108.20
1	X	2622	G	C5-C6-O6	-6.62	124.63	128.60
1	X	2481	G	N1-C6-O6	6.62	123.87	119.90
2	Y	62	C	O4'-C1'-N1	6.61	113.49	108.20
1	X	1749	G	C3'-C2'-C1'	-6.61	96.21	101.50
1	X	2585	C	C3'-C2'-C1'	-6.61	96.21	101.50
1	X	2208	U	O4'-C1'-N1	6.61	113.49	108.20
1	X	2276	C	O4'-C1'-N1	6.60	113.48	108.20
1	X	2199	C	P-O5'-C5'	6.60	131.45	120.90
1	X	1115	C	O4'-C1'-N1	6.59	113.47	108.20
1	X	537	C	N1-C2-N3	-6.59	114.58	119.20
1	X	2782	G	N9-C1'-C2'	-6.59	104.75	112.00
1	X	355	G	O4'-C1'-N9	6.59	113.47	108.20
1	X	2875	C	O4'-C1'-N1	6.59	113.47	108.20
1	X	1092	U	O4'-C1'-N1	6.58	113.47	108.20
1	X	1247	U	O4'-C1'-N1	6.58	113.46	108.20
1	X	42	G	C8-N9-C4	-6.58	103.77	106.40
1	X	131	C	O4'-C1'-N1	6.58	113.46	108.20
2	Y	75	A	P-O5'-C5'	6.57	131.42	120.90
1	X	2857	C	O4'-C1'-N1	6.57	113.46	108.20
1	X	1223	G	C4-C5-N7	6.57	113.43	110.80
1	X	1664	G	O5'-P-OP1	-6.57	99.79	105.70
1	X	1685	A	P-O3'-C3'	6.56	127.57	119.70
1	X	2475	C	O4'-C1'-N1	6.56	113.44	108.20
1	X	2492	G	O4'-C1'-N9	6.55	113.44	108.20
1	X	2596	C	O4'-C1'-N1	6.55	113.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	824	U	C1'-O4'-C4'	-6.54	104.67	109.90
1	X	1812	U	P-O3'-C3'	6.54	127.55	119.70
1	X	1333	G	N3-C4-C5	6.54	131.87	128.60
2	Y	123	U	N1-C1'-C2'	6.54	122.50	114.00
1	X	1090	C	O4'-C1'-N1	6.54	113.43	108.20
1	X	2056	C	O4'-C1'-N1	6.54	113.43	108.20
1	X	2037	A	O4'-C1'-N9	6.53	113.43	108.20
1	X	2206	C	O4'-C1'-N1	6.53	113.43	108.20
1	X	1319	C	O4'-C1'-N1	6.53	113.43	108.20
1	X	2864	C	O4'-C1'-N1	6.53	113.42	108.20
1	X	866	U	O4'-C1'-N1	6.53	113.42	108.20
1	X	1415	C	O4'-C1'-N1	6.53	113.42	108.20
1	X	1468	A	P-O5'-C5'	6.53	131.34	120.90
1	X	1939	U	N3-C2-O2	-6.53	117.63	122.20
1	X	332	C	P-O3'-C3'	6.52	127.53	119.70
1	X	2808	U	C1'-O4'-C4'	-6.52	104.68	109.90
1	X	1770	U	C5-C6-N1	-6.52	119.44	122.70
1	X	12	U	C2-N1-C1'	6.51	125.52	117.70
1	X	562	G	C3'-C2'-C1'	-6.51	96.29	101.50
1	X	1745	C	P-O3'-C3'	-6.51	111.89	119.70
1	X	2731	G	O4'-C1'-N9	6.51	113.41	108.20
1	X	1567	A	O4'-C1'-N9	6.51	113.41	108.20
1	X	1706	A	P-O5'-C5'	-6.51	110.48	120.90
1	X	2228	U	C3'-C2'-C1'	6.51	106.71	101.50
1	X	1830	C	C1'-O4'-C4'	-6.51	104.69	109.90
1	X	193	A	O4'-C1'-N9	6.50	113.40	108.20
1	X	1467	U	C5-C6-N1	6.50	125.95	122.70
2	Y	55	C	O4'-C1'-N1	6.50	113.40	108.20
1	X	1067	G	P-O3'-C3'	6.50	127.49	119.70
1	X	1009	C	N1-C2-O2	6.48	122.79	118.90
1	X	2625	U	C5-C4-O4	-6.48	122.01	125.90
1	X	2700	U	P-O3'-C3'	-6.48	111.92	119.70
1	X	182	G	P-O3'-C3'	6.48	127.47	119.70
1	X	418	C	C1'-O4'-C4'	-6.48	104.72	109.90
1	X	1764	A	C3'-C2'-C1'	-6.48	96.32	101.50
1	X	393	U	O4'-C1'-N1	6.47	113.38	108.20
1	X	1598	C	O4'-C1'-N1	6.47	113.38	108.20
2	Y	110	U	O4'-C1'-N1	6.47	113.38	108.20
1	X	689	A	C5-N7-C8	-6.47	100.67	103.90
1	X	2009	U	O4'-C1'-N1	6.47	113.37	108.20
1	X	2663	U	P-O3'-C3'	-6.47	111.94	119.70
1	X	460	U	P-O3'-C3'	6.46	127.46	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2306	A	O4'-C1'-N9	6.46	113.37	108.20
1	X	408	U	P-O3'-C3'	6.46	127.45	119.70
1	X	2671	C	N1-C2-O2	6.46	122.78	118.90
1	X	1318	A	P-O3'-C3'	6.46	127.45	119.70
1	X	1862	C	O4'-C1'-N1	6.46	113.37	108.20
1	X	1947	G	O4'-C1'-N9	-6.46	103.03	108.20
1	X	2281	C	O4'-C1'-N1	6.46	113.36	108.20
1	X	22	C	O4'-C1'-N1	6.45	113.36	108.20
1	X	2038	C	O4'-C1'-N1	6.45	113.36	108.20
2	Y	50	U	O4'-C1'-N1	6.45	113.36	108.20
1	X	873	U	O4'-C1'-N1	6.45	113.36	108.20
1	X	1223	G	C6-C5-N7	-6.45	126.53	130.40
1	X	349	G	N3-C4-C5	-6.43	125.39	128.60
1	X	1574	A	C5'-C4'-O4'	6.43	116.82	109.10
1	X	422	C	O4'-C1'-N1	6.43	113.34	108.20
1	X	1291	G	O4'-C1'-N9	6.43	113.34	108.20
1	X	1317	G	O4'-C1'-N9	6.42	113.34	108.20
1	X	1496	G	C2'-C3'-O3'	6.42	123.98	113.70
1	X	431	G	O4'-C1'-N9	6.42	113.34	108.20
1	X	446	C	N1-C2-O2	6.42	122.75	118.90
1	X	1692	C	C3'-C2'-C1'	6.42	106.64	101.50
1	X	1940	C	P-O3'-C3'	-6.42	111.99	119.70
1	X	424	G	P-O3'-C3'	6.42	127.40	119.70
1	X	2488	G	C5-C6-N1	6.42	114.71	111.50
1	X	619	A	O4'-C1'-N9	6.41	113.33	108.20
1	X	1208	A	O4'-C1'-N9	6.41	113.33	108.20
1	X	1552	C	P-O3'-C3'	6.41	127.39	119.70
1	X	559	C	C5'-C4'-C3'	6.41	126.25	116.00
1	X	1152	C	C1'-O4'-C4'	-6.41	104.78	109.90
1	X	1222	G	P-O3'-C3'	6.41	127.39	119.70
1	X	1333	G	C8-N9-C1'	6.41	135.33	127.00
1	X	244	C	O4'-C1'-N1	6.40	113.32	108.20
1	X	527	C	P-O3'-C3'	6.40	127.38	119.70
1	X	630	G	O4'-C1'-N9	6.40	113.32	108.20
2	Y	57	U	O4'-C1'-N1	6.40	113.32	108.20
1	X	956	A	P-O5'-C5'	6.39	131.13	120.90
1	X	1999	U	P-O3'-C3'	-6.39	112.03	119.70
1	X	2185	U	O4'-C1'-N1	6.39	113.32	108.20
1	X	1241	G	P-O3'-C3'	-6.39	112.03	119.70
1	X	322	A	P-O3'-C3'	6.38	127.36	119.70
1	X	429	C	O4'-C1'-N1	6.38	113.31	108.20
1	X	40	U	O4'-C1'-N1	6.38	113.31	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1229	C	N1-C2-O2	6.38	122.73	118.90
1	X	2082	C	O4'-C1'-N1	6.38	113.30	108.20
1	X	1446	U	O4'-C1'-N1	6.38	113.30	108.20
1	X	1796	A	C2-N3-C4	6.38	113.79	110.60
2	Y	17	A	O4'-C1'-N9	6.38	113.30	108.20
1	X	2032	G	C5-C6-O6	-6.38	124.78	128.60
1	X	2719	U	O4'-C1'-N1	6.38	113.30	108.20
1	X	169	C	O4'-C1'-N1	6.37	113.30	108.20
1	X	338	G	N7-C8-N9	6.37	116.29	113.10
1	X	2582	G	P-O5'-C5'	6.37	131.09	120.90
23	U	18	VAL	C-N-CA	6.37	137.63	121.70
1	X	1291	G	O4'-C4'-C3'	-6.37	97.63	104.00
1	X	1454	U	O4'-C1'-N1	6.37	113.29	108.20
1	X	1647	U	N3-C4-C5	-6.37	110.78	114.60
1	X	2032	G	O4'-C4'-C3'	-6.36	97.64	104.00
1	X	2494	C	O4'-C1'-N1	6.36	113.29	108.20
1	X	1829	C	O4'-C1'-N1	6.36	113.29	108.20
1	X	1338	G	O4'-C1'-N9	6.36	113.29	108.20
1	X	2661	G	C5-C6-O6	-6.36	124.79	128.60
1	X	2578	G	P-O5'-C5'	6.35	131.07	120.90
1	X	2653	A	O4'-C1'-N9	6.35	113.28	108.20
2	Y	86	A	C1'-O4'-C4'	-6.35	104.82	109.90
1	X	757	U	N3-C2-O2	-6.35	117.76	122.20
1	X	1670	G	O4'-C1'-N9	-6.35	103.12	108.20
1	X	1036	G	C4'-C3'-C2'	6.35	108.95	102.60
1	X	981	C	O4'-C1'-N1	6.34	113.28	108.20
1	X	1732	U	O4'-C1'-N1	6.34	113.27	108.20
1	X	309	G	C8-N9-C4	-6.34	103.86	106.40
1	X	1988	A	P-O3'-C3'	6.34	127.31	119.70
1	X	520	C	C4'-C3'-C2'	-6.34	96.26	102.60
1	X	975	C	O4'-C1'-N1	6.33	113.27	108.20
1	X	1306	U	O4'-C1'-N1	6.33	113.27	108.20
1	X	1914	U	O4'-C1'-N1	6.33	113.27	108.20
1	X	838	A	OP1-P-O3'	6.33	119.13	105.20
1	X	2772	U	O4'-C1'-N1	6.33	113.27	108.20
1	X	633	G	O4'-C1'-N9	6.33	113.26	108.20
1	X	650	U	P-O5'-C5'	6.33	131.02	120.90
1	X	967	G	P-O3'-C3'	6.32	127.29	119.70
1	X	2408	G	N3-C4-C5	-6.32	125.44	128.60
2	Y	70	C	O4'-C1'-N1	6.32	113.25	108.20
1	X	1509	A	P-O3'-C3'	6.32	127.28	119.70
1	X	1986	G	O4'-C1'-N9	6.32	113.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2544	A	O3'-P-O5'	-6.32	92.00	104.00
1	X	1044	U	P-O3'-C3'	6.31	127.28	119.70
1	X	774	A	C6-N1-C2	6.31	122.39	118.60
1	X	1392	U	P-O3'-C3'	6.31	127.27	119.70
1	X	2670	C	O4'-C1'-N1	6.31	113.25	108.20
1	X	2409	A	N9-C1'-C2'	6.31	122.20	114.00
1	X	1749	G	O4'-C1'-C2'	-6.30	99.50	105.80
1	X	2482	A	C2-N3-C4	6.30	113.75	110.60
2	Y	88	C	C1'-O4'-C4'	-6.30	104.86	109.90
1	X	1333	G	N7-C8-N9	6.30	116.25	113.10
1	X	90	G	P-O3'-C3'	6.30	127.26	119.70
1	X	98	U	O4'-C1'-N1	6.29	113.23	108.20
1	X	1017	C	O4'-C1'-N1	6.29	113.23	108.20
1	X	730	C	P-O3'-C3'	6.29	127.25	119.70
1	X	1407	G	N9-C1'-C2'	6.29	122.17	114.00
1	X	789	G	P-O3'-C3'	6.29	127.24	119.70
1	X	1236	G	C8-N9-C4	-6.29	103.89	106.40
1	X	779	U	O4'-C1'-N1	6.28	113.23	108.20
1	X	2808	U	P-O5'-C5'	6.28	130.95	120.90
2	Y	4	C	O4'-C1'-N1	6.28	113.23	108.20
1	X	343	A	N9-C1'-C2'	6.28	122.16	114.00
1	X	430	C	C6-N1-C2	-6.28	117.79	120.30
1	X	607	C	C3'-C2'-C1'	-6.28	96.48	101.50
1	X	805	G	N9-C1'-C2'	6.28	122.16	114.00
1	X	1792	C	N1-C1'-C2'	6.28	122.16	114.00
1	X	2375	G	O4'-C4'-C3'	-6.28	97.72	104.00
1	X	1982	C	O4'-C4'-C3'	-6.28	97.72	104.00
1	X	2043	A	P-O3'-C3'	6.28	127.23	119.70
19	Q	62	ARG	C-N-CA	6.27	137.38	121.70
1	X	1112	U	O4'-C1'-N1	6.27	113.22	108.20
1	X	1261	G	O4'-C1'-N9	-6.27	103.18	108.20
1	X	1689	U	P-O3'-C3'	6.27	127.23	119.70
1	X	1669	A	O4'-C4'-C3'	-6.27	97.73	104.00
1	X	1783	G	N9-C1'-C2'	-6.27	105.10	112.00
1	X	1882	G	C3'-C2'-C1'	6.27	106.52	101.50
1	X	968	C	C5'-C4'-O4'	6.26	116.61	109.10
1	X	1359	G	C5'-C4'-C3'	-6.26	105.98	116.00
1	X	1825	C	O4'-C1'-N1	6.26	113.21	108.20
1	X	2572	U	N3-C4-O4	6.26	123.78	119.40
1	X	672	C	O4'-C4'-C3'	-6.25	97.75	104.00
1	X	1522	C	N1-C2-O2	6.25	122.65	118.90
1	X	1938	U	C4'-C3'-C2'	6.25	108.85	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	456	C	O4'-C1'-N1	6.25	113.20	108.20
1	X	540	G	C5-C6-N1	6.25	114.62	111.50
1	X	655	A	C1'-O4'-C4'	-6.25	104.90	109.90
2	Y	42	U	O4'-C1'-N1	6.25	113.20	108.20
1	X	2081	U	O4'-C1'-N1	6.25	113.20	108.20
1	X	2666	U	P-O3'-C3'	6.25	127.19	119.70
1	X	1288	A	C5'-C4'-C3'	6.24	125.99	116.00
1	X	49	U	P-O3'-C3'	6.24	127.19	119.70
1	X	2258	G	O4'-C4'-C3'	-6.24	97.76	104.00
1	X	485	G	P-O3'-C3'	6.24	127.18	119.70
1	X	480	G	C5-C6-O6	-6.24	124.86	128.60
1	X	968	C	C5-C6-N1	6.24	124.12	121.00
1	X	2867	G	N7-C8-N9	6.23	116.22	113.10
1	X	517	A	P-O3'-C3'	6.23	127.17	119.70
1	X	1983	G	C3'-C2'-C1'	-6.23	96.52	101.50
1	X	2012	A	O4'-C1'-N9	6.23	113.18	108.20
1	X	2366	U	O4'-C1'-N1	6.23	113.18	108.20
1	X	2698	G	C5'-C4'-O4'	6.23	116.57	109.10
1	X	750	C	O4'-C1'-N1	6.23	113.18	108.20
1	X	79	G	C8-N9-C4	-6.22	103.91	106.40
1	X	1473	U	C4'-C3'-C2'	6.22	108.82	102.60
1	X	2667	C	C4'-C3'-C2'	-6.22	96.38	102.60
1	X	2680	U	O4'-C1'-N1	6.22	113.18	108.20
1	X	684	C	N3-C4-C5	-6.22	119.41	121.90
2	Y	90	C	C4'-C3'-C2'	6.22	108.82	102.60
1	X	1744	G	C5-C6-N1	6.21	114.61	111.50
1	X	2847	G	C8-N9-C4	-6.21	103.92	106.40
1	X	2677	U	O4'-C1'-N1	6.21	113.17	108.20
1	X	160	C	O4'-C1'-N1	6.21	113.17	108.20
1	X	699	G	C4-N9-C1'	-6.21	118.43	126.50
1	X	1190	C	O4'-C1'-N1	6.20	113.16	108.20
1	X	1230	C	O4'-C1'-N1	6.20	113.16	108.20
1	X	2717	G	O4'-C1'-N9	6.20	113.16	108.20
1	X	82	G	P-O3'-C3'	6.20	127.14	119.70
1	X	559	C	N1-C2-O2	6.20	122.62	118.90
1	X	1544	A	P-O3'-C3'	6.19	127.13	119.70
1	X	302	U	O4'-C1'-N1	6.19	113.15	108.20
1	X	2695	C	O4'-C1'-N1	6.19	113.15	108.20
1	X	725	C	O4'-C1'-N1	6.18	113.15	108.20
1	X	1819	U	O4'-C1'-N1	6.18	113.15	108.20
1	X	1412	C	C2'-C3'-O3'	6.18	123.59	113.70
1	X	699	G	C8-N9-C1'	6.18	135.03	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1947	G	P-O3'-C3'	6.18	127.12	119.70
1	X	2553	G	O4'-C1'-N9	6.18	113.14	108.20
1	X	2653	A	C3'-C2'-C1'	-6.18	96.56	101.50
1	X	1599	G	P-O3'-C3'	6.17	127.11	119.70
1	X	2500	C	O4'-C1'-N1	6.17	113.14	108.20
1	X	2507	U	O4'-C1'-N1	6.17	113.14	108.20
1	X	579	G	C5-C6-O6	6.17	132.30	128.60
1	X	942	U	N3-C2-O2	-6.17	117.88	122.20
1	X	1270	C	N3-C4-C5	-6.17	119.43	121.90
1	X	2344	G	P-O3'-C3'	6.17	127.11	119.70
2	Y	22	U	O4'-C1'-N1	6.17	113.14	108.20
2	Y	53	G	C8-N9-C4	-6.16	103.94	106.40
1	X	1056	U	P-O3'-C3'	6.16	127.09	119.70
1	X	2764	U	O4'-C1'-N1	6.16	113.13	108.20
1	X	607	C	N1-C2-O2	6.16	122.59	118.90
1	X	1570	C	P-O3'-C3'	6.16	127.09	119.70
1	X	2393	G	P-O3'-C3'	-6.15	112.32	119.70
1	X	1472	C	N1-C2-O2	6.15	122.59	118.90
2	Y	87	C	N1-C2-O2	6.15	122.59	118.90
1	X	729	A	P-O3'-C3'	6.15	127.08	119.70
1	X	940	G	C5'-C4'-O4'	6.15	116.48	109.10
1	X	2416	U	O4'-C1'-N1	6.14	113.11	108.20
1	X	631	G	P-O3'-C3'	6.14	127.07	119.70
1	X	1169	C	N1-C2-O2	6.14	122.58	118.90
1	X	1001	A	C8-N9-C4	-6.14	103.34	105.80
1	X	1128	G	P-O3'-C3'	6.13	127.06	119.70
1	X	2735	C	O4'-C1'-N1	6.13	113.11	108.20
1	X	2790	C	N1-C2-O2	6.13	122.58	118.90
2	Y	46	G	C3'-C2'-C1'	6.13	106.40	101.50
2	Y	54	U	P-O3'-C3'	6.13	127.05	119.70
1	X	539	A	N9-C1'-C2'	6.13	121.97	114.00
1	X	594	G	P-O3'-C3'	6.13	127.05	119.70
1	X	859	U	N1-C1'-C2'	6.12	121.96	114.00
1	X	933	G	P-O3'-C3'	-6.12	112.35	119.70
1	X	199	A	P-O3'-C3'	6.12	127.05	119.70
1	X	917	U	O4'-C1'-N1	6.12	113.10	108.20
1	X	2791	C	N1-C2-O2	6.12	122.57	118.90
1	X	35	G	O4'-C1'-N9	6.12	113.10	108.20
1	X	540	G	C8-N9-C4	-6.12	103.95	106.40
1	X	1824	C	N1-C2-O2	6.12	122.57	118.90
1	X	536	A	O4'-C1'-N9	6.11	113.09	108.20
1	X	1375	C	N1-C2-O2	6.11	122.57	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	19	C	O4'-C1'-N1	6.11	113.08	108.20
2	Y	45	C	N1-C2-O2	6.11	122.56	118.90
1	X	566	U	O4'-C1'-N1	6.10	113.08	108.20
1	X	1185	C	P-O5'-C5'	6.10	130.66	120.90
1	X	1325	U	O4'-C1'-N1	6.10	113.08	108.20
1	X	1647	U	N3-C4-O4	6.10	123.67	119.40
1	X	2465	G	O4'-C1'-N9	6.10	113.08	108.20
2	Y	13	C	O4'-C1'-N1	6.10	113.08	108.20
1	X	1469	U	N1-C1'-C2'	6.10	121.93	114.00
1	X	2223	U	P-O3'-C3'	-6.10	112.38	119.70
1	X	2275	U	P-O3'-C3'	6.10	127.02	119.70
1	X	2808	U	C5'-C4'-O4'	6.10	116.42	109.10
1	X	2240	C	N1-C2-O2	6.09	122.56	118.90
1	X	2415	G	P-O3'-C3'	6.09	127.01	119.70
1	X	476	G	N3-C4-C5	-6.09	125.56	128.60
1	X	875	G	C8-N9-C4	-6.09	103.97	106.40
2	Y	34	C	O4'-C1'-N1	6.08	113.07	108.20
1	X	1953	A	P-O5'-C5'	-6.08	111.17	120.90
1	X	2014	A	P-O3'-C3'	6.08	127.00	119.70
1	X	2609	G	O4'-C1'-N9	6.08	113.06	108.20
1	X	757	U	P-O3'-C3'	6.08	126.99	119.70
1	X	2315	A	O4'-C1'-N9	-6.08	103.34	108.20
1	X	1692	C	O4'-C1'-N1	6.08	113.06	108.20
1	X	1409	U	N1-C1'-C2'	6.07	121.89	114.00
1	X	2224	U	O4'-C1'-N1	6.07	113.06	108.20
1	X	2337	A	O4'-C1'-N9	6.07	113.06	108.20
2	Y	114	C	O4'-C1'-N1	6.07	113.06	108.20
1	X	955	G	P-O3'-C3'	6.07	126.98	119.70
1	X	246	C	N1-C2-O2	6.07	122.54	118.90
1	X	784	U	O4'-C1'-N1	6.07	113.05	108.20
1	X	2758	A	O4'-C1'-N9	6.07	113.05	108.20
1	X	56	C	O4'-C1'-N1	6.07	113.05	108.20
1	X	1249	G	N9-C1'-C2'	6.07	121.89	114.00
1	X	1183	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	2329	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	2869	U	O4'-C1'-N1	6.06	113.05	108.20
1	X	236	C	C6-N1-C2	-6.06	117.88	120.30
1	X	242	A	C5'-C4'-O4'	6.06	116.37	109.10
1	X	632	A	P-O3'-C3'	6.06	126.97	119.70
1	X	1986	G	P-O3'-C3'	-6.06	112.43	119.70
1	X	1773	C	N1-C2-O2	6.06	122.53	118.90
1	X	2782	G	N1-C6-O6	6.05	123.53	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	483	A	C4'-C3'-C2'	6.05	108.65	102.60
1	X	610	G	O3'-P-O5'	-6.05	92.51	104.00
1	X	2554	C	N1-C2-O2	6.04	122.53	118.90
1	X	423	G	C8-N9-C4	-6.04	103.98	106.40
1	X	794	A	N9-C1'-C2'	6.04	121.86	114.00
1	X	2795	A	C2-N3-C4	6.04	113.62	110.60
2	Y	97	C	N1-C2-O2	6.04	122.53	118.90
1	X	103	U	O4'-C1'-N1	6.04	113.03	108.20
1	X	1306	U	N3-C2-O2	-6.04	117.97	122.20
1	X	1989	C	O4'-C4'-C3'	-6.03	97.97	104.00
1	X	1388	C	O4'-C1'-N1	6.03	113.02	108.20
1	X	408	U	O4'-C1'-N1	6.03	113.02	108.20
1	X	1543	G	P-O3'-C3'	6.03	126.93	119.70
1	X	2459	C	N3-C2-O2	-6.03	117.68	121.90
1	X	1482	U	N1-C1'-C2'	6.03	121.83	114.00
1	X	2303	C	P-O3'-C3'	6.02	126.92	119.70
1	X	804	C	O4'-C1'-N1	6.02	113.01	108.20
1	X	1629	G	N9-C1'-C2'	-6.02	105.38	112.00
1	X	330	C	O4'-C1'-N1	6.01	113.01	108.20
1	X	796	A	N7-C8-N9	6.01	116.81	113.80
1	X	1594	U	O4'-C1'-N1	6.01	113.01	108.20
1	X	2178	U	O4'-C1'-N1	6.01	113.01	108.20
1	X	2840	U	P-O3'-C3'	6.01	126.92	119.70
1	X	1985	G	C3'-C2'-C1'	-6.01	96.69	101.50
1	X	2482	A	O4'-C1'-N9	6.01	113.01	108.20
1	X	2659	C	P-O3'-C3'	-6.01	112.49	119.70
1	X	343	A	P-O5'-C5'	6.00	130.51	120.90
1	X	2782	G	C5-C6-O6	-6.00	125.00	128.60
1	X	2590	U	O4'-C1'-N1	6.00	113.00	108.20
1	X	699	G	C5-N7-C8	-6.00	101.30	104.30
1	X	1217	U	C3'-C2'-C1'	-6.00	96.70	101.50
1	X	1016	C	C6-N1-C2	-5.99	117.90	120.30
2	Y	98	C	N1-C2-O2	5.99	122.50	118.90
1	X	248	A	P-O5'-C5'	5.99	130.49	120.90
1	X	1034	U	O4'-C1'-N1	5.99	112.99	108.20
1	X	2467	A	N1-C6-N6	-5.99	115.01	118.60
1	X	1407	G	C5-C6-O6	-5.99	125.01	128.60
1	X	1933	G	O4'-C1'-N9	5.99	112.99	108.20
1	X	2228	U	C6-N1-C2	-5.99	117.41	121.00
1	X	2229	G	P-O5'-C5'	-5.98	111.33	120.90
1	X	2680	U	C3'-C2'-C1'	-5.98	96.72	101.50
1	X	2688	G	O4'-C1'-N9	-5.98	103.42	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	32	C	C5-C6-N1	5.98	123.99	121.00
1	X	1030	U	O4'-C1'-N1	5.98	112.98	108.20
1	X	1284	G	N7-C8-N9	5.98	116.09	113.10
1	X	1335	A	P-O3'-C3'	-5.98	112.53	119.70
1	X	2586	G	C4'-C3'-C2'	-5.98	96.62	102.60
1	X	2808	U	C3'-C2'-C1'	-5.98	96.72	101.50
1	X	786	U	O4'-C1'-N1	5.97	112.98	108.20
1	X	1306	U	N1-C2-O2	5.97	126.98	122.80
1	X	1333	G	C5-N7-C8	-5.97	101.31	104.30
1	X	2380	U	O4'-C1'-N1	5.97	112.98	108.20
1	X	111	G	P-O5'-C5'	5.97	130.45	120.90
1	X	2724	G	O5'-C5'-C4'	-5.97	100.36	111.70
1	X	1753	A	O4'-C1'-N9	5.97	112.97	108.20
1	X	1057	A	P-O3'-C3'	5.97	126.86	119.70
1	X	1181	C	O4'-C1'-N1	5.97	112.97	108.20
1	X	1816	G	O4'-C1'-N9	5.97	112.97	108.20
1	X	675	C	C3'-C2'-C1'	-5.96	96.73	101.50
1	X	1526	U	P-O5'-C5'	5.96	130.44	120.90
1	X	1076	U	O4'-C1'-N1	5.96	112.97	108.20
1	X	1339	U	OP2-P-O3'	5.96	118.31	105.20
1	X	1249	G	C2'-C3'-O3'	5.96	123.23	113.70
1	X	1338	G	N3-C4-N9	5.96	129.57	126.00
1	X	2598	C	N1-C2-O2	5.96	122.47	118.90
1	X	1978	U	C5-C4-O4	-5.96	122.33	125.90
1	X	2672	U	N3-C2-O2	-5.96	118.03	122.20
1	X	1744	G	N3-C4-N9	5.96	129.57	126.00
1	X	2867	G	C5-N7-C8	-5.96	101.32	104.30
1	X	560	G	N9-C1'-C2'	5.95	121.74	114.00
1	X	1111	C	O4'-C1'-N1	5.95	112.96	108.20
1	X	2561	G	C6-C5-N7	-5.95	126.83	130.40
1	X	2708	U	O4'-C1'-N1	5.95	112.96	108.20
1	X	2649	A	C5'-C4'-C3'	-5.94	106.49	116.00
1	X	1142	G	O4'-C1'-C2'	-5.94	99.86	105.80
2	Y	35	C	O4'-C1'-N1	5.94	112.95	108.20
1	X	1582	A	C5'-C4'-O4'	5.94	116.23	109.10
1	X	1647	U	O4'-C1'-N1	5.94	112.95	108.20
1	X	2837	G	P-O3'-C3'	-5.94	112.57	119.70
1	X	852	U	P-O5'-C5'	-5.93	111.41	120.90
1	X	2616	U	O4'-C1'-N1	5.93	112.95	108.20
1	X	1439	G	C2'-C3'-O3'	5.93	123.19	113.70
1	X	2835	A	N1-C6-N6	5.93	122.16	118.60
1	X	580	A	C1'-O4'-C4'	-5.93	105.16	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1708	C	O4'-C1'-N1	5.93	112.94	108.20
1	X	2769	C	P-O3'-C3'	5.93	126.81	119.70
1	X	957	G	C5-C6-N1	5.93	114.46	111.50
1	X	2523	G	O4'-C1'-N9	5.93	112.94	108.20
1	X	1939	U	N1-C2-O2	5.93	126.95	122.80
1	X	2839	G	C5-C6-N1	5.93	114.46	111.50
1	X	1099	A	P-O3'-C3'	5.92	126.81	119.70
1	X	2201	G	C5'-C4'-O4'	5.92	116.21	109.10
1	X	1245	G	O4'-C1'-N9	5.92	112.94	108.20
1	X	2338	C	O4'-C1'-N1	5.92	112.93	108.20
2	Y	7	C	O4'-C1'-N1	5.92	112.93	108.20
1	X	938	G	C3'-C2'-C1'	5.91	106.23	101.50
1	X	2013	A	C5'-C4'-O4'	5.91	116.20	109.10
1	X	827	C	O4'-C1'-N1	5.91	112.93	108.20
1	X	26	G	C8-N9-C4	-5.91	104.03	106.40
1	X	334	G	O4'-C1'-N9	5.91	112.93	108.20
1	X	468	A	P-O3'-C3'	5.91	126.79	119.70
1	X	2493	U	O4'-C1'-N1	5.91	112.93	108.20
2	Y	49	C	C5'-C4'-O4'	5.90	116.18	109.10
1	X	2359	U	O4'-C1'-N1	5.90	112.92	108.20
1	X	540	G	C5-C6-O6	5.90	132.14	128.60
1	X	1744	G	N3-C4-C5	-5.90	125.65	128.60
1	X	2599	U	P-O5'-C5'	-5.90	111.47	120.90
1	X	1678	G	C5-C6-O6	-5.90	125.06	128.60
1	X	2015	G	N9-C1'-C2'	5.90	121.67	114.00
1	X	2444	C	O4'-C1'-N1	5.89	112.91	108.20
1	X	2636	A	O4'-C1'-N9	5.89	112.92	108.20
1	X	884	C	O4'-C1'-N1	5.89	112.91	108.20
1	X	1529	C	O4'-C1'-N1	5.89	112.91	108.20
1	X	657	A	C3'-C2'-C1'	-5.89	96.79	101.50
1	X	2017	U	O4'-C1'-N1	5.89	112.91	108.20
15	M	29	PRO	N-CA-C	5.89	127.41	112.10
1	X	1454	U	N3-C4-O4	5.88	123.52	119.40
1	X	2441	U	O4'-C1'-N1	5.88	112.90	108.20
1	X	1089	C	P-O3'-C3'	5.88	126.75	119.70
1	X	1244	U	C5-C6-N1	5.87	125.64	122.70
1	X	2572	U	O4'-C1'-N1	5.87	112.90	108.20
1	X	882	C	N1-C2-O2	5.87	122.42	118.90
1	X	1736	C	O4'-C1'-N1	5.87	112.90	108.20
1	X	155	G	O4'-C1'-N9	5.87	112.90	108.20
1	X	1429	A	P-O3'-C3'	5.87	126.74	119.70
1	X	237	G	O4'-C1'-N9	5.87	112.89	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	559	C	N3-C2-O2	-5.87	117.79	121.90
1	X	999	A	O4'-C1'-N9	5.87	112.89	108.20
1	X	2619	G	C5-C6-O6	-5.87	125.08	128.60
1	X	1678	G	O4'-C4'-C3'	-5.86	98.14	104.00
1	X	1023	U	P-O3'-C3'	5.86	126.73	119.70
1	X	2225	G	O4'-C1'-N9	5.86	112.89	108.20
1	X	2560	G	C3'-C2'-C1'	5.86	106.19	101.50
1	X	2745	A	P-O3'-C3'	5.86	126.73	119.70
1	X	2370	G	C1'-O4'-C4'	-5.86	105.21	109.90
1	X	1627	C	O4'-C1'-N1	5.86	112.89	108.20
1	X	939	C	C3'-C2'-C1'	5.85	106.18	101.50
1	X	998	C	O4'-C1'-N1	5.85	112.88	108.20
2	Y	2	C	O4'-C1'-N1	5.85	112.88	108.20
1	X	234	C	O4'-C1'-N1	5.85	112.88	108.20
1	X	771	C	C4'-C3'-C2'	-5.85	96.75	102.60
1	X	1353	A	O4'-C1'-N9	5.85	112.88	108.20
1	X	1667	A	N1-C6-N6	5.85	122.11	118.60
1	X	2797	G	P-O3'-C3'	5.85	126.72	119.70
2	Y	76	U	O4'-C1'-N1	5.85	112.88	108.20
1	X	577	U	C1'-O4'-C4'	-5.85	105.22	109.90
1	X	2797	G	N3-C4-N9	5.85	129.51	126.00
1	X	1389	C	O4'-C1'-N1	5.85	112.88	108.20
1	X	1975	G	N1-C6-O6	-5.84	116.39	119.90
1	X	2635	U	O4'-C1'-N1	5.84	112.88	108.20
1	X	2303	C	N1-C2-O2	5.84	122.41	118.90
1	X	2376	G	P-O5'-C5'	5.84	130.24	120.90
1	X	2009	U	P-O3'-C3'	-5.84	112.69	119.70
9	G	106	TYR	N-CA-CB	5.84	121.11	110.60
2	Y	116	C	O4'-C1'-N1	5.84	112.87	108.20
1	X	68	C	N1-C2-O2	5.83	122.40	118.90
1	X	422	C	C6-N1-C2	-5.83	117.97	120.30
1	X	741	G	P-O3'-C3'	5.83	126.70	119.70
1	X	1888	C	C3'-C2'-C1'	5.83	106.16	101.50
1	X	770	U	C3'-C2'-C1'	-5.83	96.84	101.50
1	X	1223	G	C5-C6-O6	-5.83	125.11	128.60
1	X	2645	C	O4'-C1'-N1	5.83	112.86	108.20
1	X	434	C	O4'-C1'-N1	5.82	112.86	108.20
1	X	522	G	N9-C1'-C2'	5.82	121.57	114.00
1	X	1993	G	C8-N9-C4	-5.82	104.07	106.40
1	X	2627	G	C5-C6-O6	-5.82	125.11	128.60
1	X	1032	A	C3'-C2'-C1'	-5.82	96.84	101.50
1	X	575	U	O4'-C1'-N1	5.82	112.86	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1682	A	C5-C6-N6	-5.82	119.05	123.70
1	X	2567	G	N7-C8-N9	5.82	116.01	113.10
1	X	533	C	O4'-C1'-N1	5.81	112.85	108.20
1	X	1778	U	O4'-C1'-N1	5.81	112.85	108.20
1	X	2797	G	C6-C5-N7	-5.81	126.92	130.40
1	X	797	A	P-O3'-C3'	5.80	126.67	119.70
1	X	220	U	O4'-C1'-N1	5.80	112.84	108.20
1	X	689	A	N7-C8-N9	5.80	116.70	113.80
1	X	582	G	C8-N9-C4	-5.80	104.08	106.40
1	X	339	U	C3'-C2'-C1'	5.80	106.14	101.50
1	X	1831	G	C8-N9-C4	-5.80	104.08	106.40
1	X	661	C	N1-C2-O2	5.79	122.38	118.90
1	X	2460	G	C8-N9-C4	-5.79	104.08	106.40
1	X	1407	G	C8-N9-C4	-5.79	104.08	106.40
1	X	1276	U	O4'-C1'-N1	5.79	112.83	108.20
1	X	466	A	P-O3'-C3'	5.79	126.64	119.70
1	X	1058	G	O4'-C1'-N9	5.79	112.83	108.20
1	X	1466	C	C4'-C3'-C2'	-5.79	96.81	102.60
1	X	1920	A	C1'-O4'-C4'	-5.79	105.27	109.90
1	X	2230	G	C5'-C4'-O4'	-5.79	102.16	109.10
1	X	2778	U	C3'-C2'-C1'	5.79	106.13	101.50
1	X	541	C	P-O3'-C3'	5.78	126.64	119.70
1	X	1987	G	C5-C6-O6	-5.78	125.13	128.60
1	X	556	A	P-O3'-C3'	5.78	126.64	119.70
1	X	461	A	C2-N3-C4	5.78	113.49	110.60
1	X	774	A	C4-C5-C6	5.78	119.89	117.00
1	X	1286	U	P-O3'-C3'	5.78	126.63	119.70
1	X	2527	G	C8-N9-C4	-5.78	104.09	106.40
1	X	467	U	N3-C2-O2	-5.78	118.16	122.20
1	X	1122	A	N9-C1'-C2'	5.78	121.51	114.00
1	X	1288	A	P-O3'-C3'	-5.77	112.77	119.70
1	X	1958	G	C5-C6-N1	5.77	114.39	111.50
1	X	1753	A	P-O5'-C5'	5.77	130.13	120.90
1	X	2487	G	C5-C6-N1	5.77	114.39	111.50
1	X	2604	G	C5-C6-N1	5.77	114.39	111.50
2	Y	64	C	O4'-C1'-N1	5.77	112.82	108.20
1	X	2571	G	C3'-C2'-C1'	-5.77	96.89	101.50
1	X	1224	A	P-O3'-C3'	5.76	126.62	119.70
1	X	202	A	O4'-C1'-N9	5.76	112.81	108.20
1	X	1058	G	C1'-O4'-C4'	-5.76	105.29	109.90
1	X	1841	G	O4'-C1'-N9	5.76	112.81	108.20
1	X	673	G	C2'-C3'-O3'	5.76	122.92	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1811	A	C2'-C3'-O3'	5.76	122.92	113.70
2	Y	76	U	N3-C2-O2	-5.76	118.17	122.20
1	X	29	U	O4'-C1'-N1	5.76	112.81	108.20
1	X	396	U	C1'-O4'-C4'	-5.76	105.30	109.90
1	X	764	A	O5'-P-OP2	-5.76	100.52	105.70
1	X	2840	U	O4'-C1'-N1	5.75	112.80	108.20
1	X	1311	C	N1-C2-O2	5.75	122.35	118.90
1	X	1251	G	N9-C1'-C2'	-5.75	105.68	112.00
2	Y	5	C	O4'-C1'-N1	5.75	112.80	108.20
1	X	352	G	P-O5'-C5'	5.74	130.09	120.90
1	X	603	C	N1-C2-O2	5.74	122.34	118.90
1	X	2458	U	O4'-C1'-N1	5.74	112.79	108.20
1	X	223	C	P-O3'-C3'	-5.74	112.81	119.70
1	X	1843	U	O4'-C1'-N1	5.74	112.79	108.20
1	X	2427	A	P-O3'-C3'	5.74	126.58	119.70
1	X	1081	A	P-O3'-C3'	5.74	126.58	119.70
1	X	420	C	O4'-C1'-N1	5.74	112.79	108.20
1	X	447	U	P-O3'-C3'	5.74	126.58	119.70
1	X	1729	C	O4'-C1'-N1	5.74	112.79	108.20
1	X	2572	U	C3'-C2'-C1'	-5.73	96.91	101.50
1	X	2735	C	C6-N1-C2	-5.73	118.01	120.30
1	X	67	G	O4'-C1'-N9	5.73	112.78	108.20
1	X	1442	C	N1-C2-O2	5.73	122.34	118.90
1	X	2364	C	O4'-C1'-N1	5.73	112.78	108.20
1	X	799	C	P-O5'-C5'	-5.72	111.74	120.90
1	X	860	U	C5'-C4'-O4'	5.72	115.97	109.10
1	X	2048	C	P-O5'-C5'	-5.72	111.75	120.90
1	X	2559	U	N1-C2-O2	5.72	126.80	122.80
1	X	2573	C	O4'-C1'-N1	5.72	112.78	108.20
1	X	574	C	P-O3'-C3'	-5.71	112.84	119.70
1	X	1394	G	O4'-C1'-N9	5.71	112.77	108.20
1	X	12	U	N3-C2-O2	-5.71	118.20	122.20
1	X	1093	U	O4'-C1'-N1	5.71	112.77	108.20
1	X	2018	G	C5'-C4'-C3'	-5.71	106.86	116.00
1	X	2724	G	P-O5'-C5'	5.71	130.04	120.90
2	Y	109	G	O4'-C1'-N9	5.71	112.77	108.20
1	X	421	G	P-O5'-C5'	5.71	130.03	120.90
1	X	474	G	O4'-C1'-N9	5.71	112.77	108.20
1	X	536	A	P-O3'-C3'	5.71	126.55	119.70
1	X	724	C	O4'-C1'-N1	5.71	112.77	108.20
1	X	2876	C	O4'-C1'-N1	5.71	112.77	108.20
1	X	1635	G	P-O3'-C3'	-5.70	112.86	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	924	C	N1-C2-O2	5.70	122.32	118.90
1	X	2277	A	O4'-C1'-N9	5.70	112.76	108.20
1	X	2075	U	P-O3'-C3'	5.70	126.54	119.70
1	X	464	G	C3'-C2'-C1'	5.70	106.06	101.50
1	X	1490	U	O4'-C1'-N1	5.70	112.76	108.20
1	X	2258	G	C1'-O4'-C4'	-5.70	105.34	109.90
1	X	2235	G	C3'-C2'-C1'	-5.69	96.94	101.50
2	Y	83	C	N1-C2-O2	5.69	122.32	118.90
1	X	1570	C	N1-C2-O2	5.69	122.31	118.90
1	X	2552	C	O3'-P-O5'	-5.69	93.19	104.00
1	X	516	G	C5-C6-O6	-5.69	125.19	128.60
1	X	656	U	P-O5'-C5'	5.69	130.00	120.90
1	X	2015	G	N7-C8-N9	5.69	115.94	113.10
1	X	1518	C	O4'-C1'-N1	5.68	112.75	108.20
2	Y	120	G	O4'-C1'-N9	5.68	112.75	108.20
1	X	1668	G	P-O5'-C5'	5.68	129.99	120.90
1	X	2702	G	C6-C5-N7	-5.68	126.99	130.40
1	X	156	G	C3'-C2'-C1'	-5.68	96.96	101.50
1	X	889	C	O4'-C1'-N1	5.68	112.74	108.20
1	X	689	A	N1-C6-N6	5.67	122.00	118.60
1	X	2715	C	O4'-C1'-N1	5.67	112.74	108.20
1	X	34	U	C2-N1-C1'	5.67	124.51	117.70
1	X	1341	G	C4'-C3'-C2'	5.67	108.27	102.60
1	X	2846	G	O4'-C1'-N9	5.67	112.74	108.20
15	M	28	ARG	N-CA-C	-5.67	95.69	111.00
1	X	490	A	C5'-C4'-O4'	5.67	115.90	109.10
1	X	2245	A	C5'-C4'-O4'	5.67	115.90	109.10
1	X	467	U	N1-C2-O2	5.67	126.77	122.80
1	X	1075	C	O4'-C1'-N1	5.67	112.73	108.20
1	X	225	G	O4'-C1'-N9	5.67	112.73	108.20
1	X	1222	G	N3-C4-C5	-5.67	125.77	128.60
1	X	1500	U	O4'-C1'-N1	5.66	112.73	108.20
1	X	2285	U	O4'-C1'-N1	5.66	112.73	108.20
1	X	1237	G	O4'-C1'-N9	5.66	112.73	108.20
1	X	1415	C	N1-C2-O2	5.66	122.30	118.90
1	X	1570	C	N3-C2-O2	-5.66	117.94	121.90
1	X	2013	A	C1'-O4'-C4'	-5.66	105.37	109.90
1	X	1324	G	O4'-C1'-C2'	-5.66	100.14	105.80
1	X	2671	C	C4'-C3'-C2'	-5.66	96.94	102.60
1	X	454	G	C4'-C3'-C2'	5.66	108.26	102.60
1	X	478	G	P-O3'-C3'	-5.65	112.92	119.70
1	X	1252	C	C5-C6-N1	5.65	123.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2300	G	O4'-C1'-N9	5.65	112.72	108.20
1	X	413	G	O4'-C1'-N9	5.65	112.72	108.20
1	X	459	A	P-O3'-C3'	5.65	126.48	119.70
1	X	1159	U	O4'-C1'-N1	5.65	112.72	108.20
1	X	1281	A	OP2-P-O3'	5.65	117.63	105.20
1	X	516	G	P-O3'-C3'	5.65	126.48	119.70
1	X	1277	G	N3-C4-C5	-5.65	125.78	128.60
1	X	915	C	O4'-C1'-N1	5.64	112.72	108.20
1	X	1421	U	O4'-C1'-N1	5.64	112.72	108.20
1	X	1700	C	P-O3'-C3'	-5.64	112.93	119.70
1	X	175	C	C5-C6-N1	5.64	123.82	121.00
1	X	2018	G	N3-C4-C5	5.64	131.42	128.60
1	X	2552	C	O4'-C1'-N1	5.64	112.71	108.20
1	X	21	A	P-O3'-C3'	-5.64	112.93	119.70
1	X	1337	G	C3'-C2'-C1'	-5.64	96.99	101.50
1	X	2791	C	N3-C2-O2	-5.64	117.95	121.90
1	X	2545	A	P-O3'-C3'	5.64	126.46	119.70
1	X	219	G	O4'-C1'-N9	-5.63	103.69	108.20
1	X	2296	U	O4'-C1'-N1	5.63	112.71	108.20
1	X	42	G	N7-C8-N9	5.63	115.92	113.10
1	X	742	G	C5'-C4'-O4'	5.63	115.86	109.10
1	X	2075	U	O4'-C1'-N1	5.63	112.71	108.20
1	X	2353	G	N3-C4-C5	-5.63	125.78	128.60
1	X	1683	G	O4'-C1'-N9	5.63	112.70	108.20
1	X	1753	A	N7-C8-N9	5.63	116.61	113.80
1	X	806	A	P-O3'-C3'	5.62	126.45	119.70
1	X	426	C	O4'-C1'-N1	5.62	112.70	108.20
1	X	2559	U	P-O3'-C3'	5.62	126.44	119.70
1	X	12	U	N1-C2-O2	5.62	126.73	122.80
1	X	1229	C	O4'-C1'-N1	5.62	112.69	108.20
1	X	75	C	O4'-C1'-N1	5.62	112.69	108.20
1	X	168	A	O4'-C1'-N9	5.62	112.69	108.20
1	X	746	G	N3-C4-C5	-5.62	125.79	128.60
1	X	749	C	C5-C6-N1	5.62	123.81	121.00
1	X	190	A	O4'-C4'-C3'	-5.61	98.39	104.00
1	X	540	G	N9-C1'-C2'	5.61	121.30	114.00
1	X	2294	U	P-O3'-C3'	5.61	126.43	119.70
1	X	2782	G	C6-C5-N7	-5.61	127.03	130.40
1	X	1201	G	C8-N9-C4	-5.61	104.16	106.40
1	X	1249	G	N1-C6-O6	-5.61	116.54	119.90
1	X	2652	G	N3-C4-C5	-5.61	125.80	128.60
1	X	2541	U	N3-C2-O2	-5.60	118.28	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	690	A	P-O3'-C3'	5.60	126.42	119.70
1	X	1037	U	O4'-C1'-N1	5.60	112.68	108.20
1	X	2033	C	N1-C2-O2	5.60	122.26	118.90
1	X	1086	C	C3'-C2'-C1'	5.60	105.98	101.50
1	X	1314	A	O4'-C1'-C2'	-5.60	100.20	105.80
1	X	746	G	N3-C4-N9	5.60	129.36	126.00
1	X	982	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	1399	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	1341	G	C5-C6-N1	5.60	114.30	111.50
1	X	1411	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	1660	G	O4'-C1'-N9	5.60	112.68	108.20
1	X	441	A	P-O3'-C3'	5.60	126.42	119.70
1	X	1607	A	C2'-C3'-O3'	5.59	122.65	113.70
1	X	169	C	N1-C2-O2	5.59	122.25	118.90
1	X	392	G	P-O3'-C3'	-5.59	112.99	119.70
1	X	1257	U	O4'-C1'-N1	5.59	112.67	108.20
1	X	534	U	O4'-C1'-N1	5.59	112.67	108.20
1	X	555	U	C1'-O4'-C4'	-5.59	105.43	109.90
1	X	927	C	N3-C2-O2	-5.59	117.99	121.90
1	X	13	A	P-O3'-C3'	5.59	126.41	119.70
1	X	1986	G	O5'-P-OP2	-5.59	100.67	105.70
12	J	87	GLY	C-N-CA	5.59	135.67	121.70
1	X	327	C	N1-C2-O2	5.59	122.25	118.90
1	X	1528	C	O4'-C1'-N1	5.59	112.67	108.20
1	X	1439	G	C8-N9-C4	-5.58	104.17	106.40
1	X	1922	U	P-O3'-C3'	5.58	126.40	119.70
2	Y	14	C	N1-C2-O2	5.58	122.25	118.90
1	X	165	G	O4'-C1'-N9	5.58	112.67	108.20
1	X	719	A	P-O3'-C3'	5.58	126.40	119.70
1	X	1304	U	O4'-C1'-N1	5.58	112.66	108.20
1	X	204	A	C2'-C3'-O3'	5.58	122.63	113.70
1	X	1636	G	O4'-C1'-N9	5.58	112.66	108.20
1	X	1087	C	O4'-C1'-N1	5.58	112.66	108.20
1	X	2338	C	N1-C2-O2	5.58	122.25	118.90
1	X	2403	C	N3-C2-O2	-5.58	118.00	121.90
1	X	327	C	P-O3'-C3'	-5.58	113.01	119.70
1	X	2421	C	O4'-C1'-N1	5.57	112.66	108.20
1	X	2527	G	C2-N3-C4	5.57	114.69	111.90
1	X	1010	U	C5'-C4'-O4'	5.57	115.79	109.10
1	X	2228	U	C4-C5-C6	5.57	123.04	119.70
1	X	878	C	O4'-C1'-N1	5.57	112.66	108.20
2	Y	54	U	C3'-C2'-C1'	5.57	105.96	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2015	G	C8-N9-C4	-5.57	104.17	106.40
1	X	2321	C	O4'-C1'-N1	5.57	112.66	108.20
1	X	2435	C	P-O3'-C3'	-5.57	113.02	119.70
1	X	2470	U	P-O3'-C3'	5.57	126.38	119.70
2	Y	32	C	O4'-C1'-N1	5.57	112.65	108.20
1	X	687	G	C3'-C2'-C1'	-5.57	97.05	101.50
1	X	541	C	N1-C1'-C2'	5.56	121.23	114.00
1	X	842	A	C1'-O4'-C4'	-5.56	105.45	109.90
1	X	70	A	P-O3'-C3'	5.56	126.38	119.70
1	X	162	C	O4'-C1'-N1	5.56	112.65	108.20
1	X	617	U	C2-N1-C1'	5.56	124.38	117.70
1	X	2047	C	O4'-C1'-N1	5.56	112.65	108.20
1	X	2791	C	O4'-C1'-N1	5.56	112.65	108.20
1	X	2748	C	O4'-C1'-N1	5.56	112.65	108.20
1	X	2821	G	O4'-C1'-N9	5.56	112.65	108.20
1	X	1630	A	C8-N9-C4	-5.56	103.58	105.80
1	X	1771	A	N1-C6-N6	5.56	121.94	118.60
1	X	2444	C	N1-C2-O2	5.56	122.23	118.90
1	X	2702	G	N7-C8-N9	5.56	115.88	113.10
1	X	2459	C	O4'-C1'-N1	5.56	112.64	108.20
1	X	2668	U	C5-C4-O4	5.56	129.23	125.90
1	X	1593	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	2016	A	N1-C2-N3	-5.55	126.52	129.30
1	X	2422	C	N3-C2-O2	-5.55	118.01	121.90
1	X	1858	C	N1-C2-O2	5.55	122.23	118.90
1	X	86	U	C3'-C2'-C1'	-5.55	97.06	101.50
1	X	1182	U	O4'-C1'-N1	5.55	112.64	108.20
1	X	1251	G	O4'-C1'-N9	5.55	112.64	108.20
1	X	1506	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	467	U	O4'-C1'-N1	5.54	112.64	108.20
1	X	957	G	N3-C4-C5	-5.54	125.83	128.60
1	X	398	C	P-O5'-C5'	5.54	129.76	120.90
1	X	1850	G	O4'-C1'-N9	5.54	112.63	108.20
1	X	2367	A	O4'-C1'-N9	5.54	112.63	108.20
1	X	562	G	O4'-C4'-C3'	-5.54	98.46	104.00
1	X	956	A	C5'-C4'-O4'	5.54	115.74	109.10
1	X	537	C	C6-N1-C1'	-5.54	114.16	120.80
1	X	1275	A	P-O5'-C5'	5.54	129.76	120.90
1	X	1533	G	C5-C6-O6	-5.54	125.28	128.60
1	X	2321	C	C6-N1-C2	-5.54	118.09	120.30
1	X	2775	U	P-O3'-C3'	5.54	126.34	119.70
1	X	224	G	C3'-C2'-C1'	5.53	105.92	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	236	C	N1-C2-O2	5.53	122.22	118.90
1	X	2204	A	C5'-C4'-O4'	5.53	115.74	109.10
1	X	156	G	P-O3'-C3'	-5.53	113.07	119.70
1	X	640	C	O4'-C1'-N1	5.53	112.62	108.20
1	X	1142	G	N3-C4-N9	5.53	129.31	126.00
1	X	1630	A	P-O3'-C3'	-5.53	113.07	119.70
1	X	1829	C	P-O3'-C3'	-5.53	113.07	119.70
1	X	2315	A	P-O3'-C3'	5.53	126.33	119.70
1	X	612	G	O4'-C1'-N9	5.52	112.62	108.20
1	X	632	A	C4'-C3'-C2'	-5.52	97.08	102.60
1	X	1233	A	P-O3'-C3'	5.52	126.32	119.70
1	X	1539	U	O4'-C1'-N1	5.52	112.61	108.20
1	X	2496	C	O4'-C1'-N1	5.52	112.61	108.20
1	X	919	U	N1-C2-O2	5.52	126.66	122.80
1	X	1280	U	N3-C2-O2	-5.52	118.34	122.20
1	X	1707	A	P-O3'-C3'	5.52	126.32	119.70
1	X	682	G	C5-C6-N1	5.51	114.26	111.50
1	X	1626	A	N1-C2-N3	-5.51	126.54	129.30
1	X	1840	A	O4'-C1'-N9	5.51	112.61	108.20
1	X	1912	G	P-O3'-C3'	5.51	126.32	119.70
1	X	2222	U	P-O5'-C5'	5.51	129.72	120.90
1	X	440	U	O4'-C1'-N1	5.51	112.61	108.20
1	X	1447	U	O4'-C1'-N1	5.51	112.61	108.20
1	X	455	A	O4'-C1'-N9	5.51	112.61	108.20
1	X	2591	C	N1-C2-N3	-5.51	115.34	119.20
2	Y	10	U	O4'-C1'-N1	5.51	112.61	108.20
1	X	632	A	C1'-O4'-C4'	-5.51	105.49	109.90
1	X	689	A	O4'-C1'-N9	5.51	112.61	108.20
1	X	565	A	P-O3'-C3'	-5.51	113.09	119.70
1	X	2863	U	O4'-C1'-N1	5.50	112.60	108.20
1	X	1167	A	O4'-C1'-N9	-5.50	103.80	108.20
1	X	2620	G	C5-C6-O6	-5.50	125.30	128.60
1	X	2782	G	O4'-C4'-C3'	-5.50	98.50	104.00
1	X	770	U	P-O3'-C3'	-5.50	113.10	119.70
1	X	1225	G	N3-C4-C5	-5.50	125.85	128.60
1	X	1289	A	O4'-C4'-C3'	-5.50	98.50	104.00
1	X	1936	A	N1-C2-N3	-5.50	126.55	129.30
2	Y	55	C	P-O3'-C3'	5.50	126.30	119.70
1	X	1337	G	O4'-C1'-N9	5.50	112.60	108.20
1	X	1743	C	O4'-C1'-N1	5.50	112.60	108.20
1	X	1976	U	C3'-C2'-C1'	5.50	105.90	101.50
1	X	738	G	C8-N9-C4	-5.50	104.20	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2088	U	O4'-C1'-N1	5.50	112.60	108.20
1	X	2589	C	N1-C1'-C2'	5.50	121.14	114.00
1	X	476	G	O4'-C1'-N9	5.49	112.59	108.20
1	X	859	U	C5'-C4'-O4'	5.49	115.69	109.10
1	X	1294	G	C4'-C3'-C2'	-5.49	97.11	102.60
1	X	2628	C	C3'-C2'-C1'	-5.49	97.11	101.50
1	X	1162	A	O4'-C1'-N9	5.49	112.59	108.20
1	X	521	U	C2-N1-C1'	5.49	124.29	117.70
1	X	2382	C	O4'-C1'-N1	5.49	112.59	108.20
1	X	1782	A	P-O5'-C5'	5.49	129.68	120.90
1	X	2528	G	OP1-P-O3'	5.49	117.27	105.20
1	X	1831	G	O4'-C1'-N9	5.48	112.59	108.20
1	X	2184	C	O4'-C1'-N1	5.48	112.58	108.20
1	X	2496	C	O3'-P-O5'	-5.48	93.58	104.00
1	X	2528	G	N3-C4-C5	-5.48	125.86	128.60
1	X	796	A	C4-C5-N7	5.48	113.44	110.70
2	Y	112	A	O4'-C1'-N9	5.48	112.58	108.20
23	U	33	LYS	C-N-CA	5.48	135.40	121.70
1	X	322	A	O4'-C1'-N9	5.48	112.58	108.20
1	X	540	G	N9-C4-C5	5.48	107.59	105.40
1	X	698	A	C1'-O4'-C4'	-5.48	105.52	109.90
1	X	940	G	C4'-C3'-C2'	-5.48	97.12	102.60
1	X	1456	C	O4'-C1'-N1	5.48	112.58	108.20
2	Y	76	U	N1-C2-O2	5.48	126.63	122.80
1	X	973	U	O3'-P-O5'	-5.48	93.59	104.00
1	X	2196	U	O4'-C1'-N1	5.48	112.58	108.20
1	X	707	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	1469	U	C5'-C4'-O4'	5.47	115.67	109.10
1	X	1672	A	C3'-C2'-C1'	-5.47	97.12	101.50
1	X	2552	C	OP1-P-O3'	5.47	117.24	105.20
1	X	613	A	P-O3'-C3'	5.47	126.27	119.70
1	X	1308	C	C4'-C3'-C2'	-5.47	97.13	102.60
1	X	1808	C	N1-C2-O2	5.47	122.18	118.90
1	X	2330	G	C8-N9-C4	-5.47	104.21	106.40
1	X	2494	C	N3-C2-O2	-5.47	118.07	121.90
1	X	1965	U	N1-C2-O2	5.47	126.63	122.80
1	X	467	U	C2-N1-C1'	5.47	124.26	117.70
1	X	557	U	N1-C1'-C2'	5.47	121.11	114.00
1	X	1550	C	O4'-C1'-N1	5.47	112.58	108.20
1	X	1688	U	C5-C6-N1	5.47	125.43	122.70
1	X	165	G	C8-N9-C4	-5.46	104.21	106.40
1	X	1473	U	O4'-C1'-C2'	5.46	112.52	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2876	C	P-O3'-C3'	5.46	126.26	119.70
1	X	1142	G	N3-C4-C5	-5.46	125.87	128.60
1	X	535	U	O4'-C1'-N1	5.46	112.57	108.20
1	X	1664	G	P-O5'-C5'	5.46	129.64	120.90
1	X	1767	G	O4'-C1'-N9	5.46	112.57	108.20
1	X	2443	C	O4'-C1'-N1	5.46	112.57	108.20
1	X	241	C	N1-C2-O2	5.46	122.17	118.90
1	X	1381	G	C8-N9-C4	-5.46	104.22	106.40
1	X	1663	C	OP1-P-O3'	5.46	117.21	105.20
1	X	2587	G	O4'-C1'-N9	5.46	112.57	108.20
1	X	358	C	C6-N1-C2	-5.46	118.12	120.30
1	X	979	A	O4'-C1'-N9	5.46	112.56	108.20
1	X	1235	C	C5-C6-N1	5.46	123.73	121.00
1	X	1439	G	N7-C8-N9	5.46	115.83	113.10
1	X	1715	A	P-O3'-C3'	5.46	126.25	119.70
1	X	2540	A	N9-C1'-C2'	-5.46	106.00	112.00
1	X	520	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	1882	G	P-O5'-C5'	5.45	129.62	120.90
1	X	2539	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	2330	G	P-O3'-C3'	5.45	126.24	119.70
2	Y	30	C	P-O5'-C5'	5.45	129.62	120.90
1	X	429	C	N1-C2-O2	5.45	122.17	118.90
1	X	1146	G	P-O3'-C3'	-5.44	113.17	119.70
1	X	11	G	C8-N9-C4	-5.44	104.22	106.40
1	X	144	U	O4'-C1'-N1	5.44	112.55	108.20
1	X	1766	U	P-O5'-C5'	-5.44	112.19	120.90
1	X	2268	G	O4'-C1'-N9	5.44	112.55	108.20
1	X	1924	C	N1-C2-O2	5.44	122.17	118.90
1	X	2734	U	O4'-C1'-N1	5.44	112.55	108.20
1	X	1254	G	C8-N9-C4	-5.44	104.22	106.40
1	X	227	G	P-O3'-C3'	5.44	126.22	119.70
1	X	2668	U	C5-C6-N1	-5.44	119.98	122.70
1	X	1219	C	C5-C6-N1	5.44	123.72	121.00
1	X	1466	C	N1-C2-O2	5.43	122.16	118.90
1	X	2608	A	N9-C1'-C2'	5.43	121.06	114.00
1	X	2854	G	O4'-C1'-C2'	-5.43	100.36	105.80
1	X	191	G	C8-N9-C4	-5.43	104.23	106.40
1	X	458	G	C3'-C2'-C1'	5.43	105.85	101.50
1	X	579	G	N9-C4-C5	5.43	107.57	105.40
1	X	1680	U	P-O3'-C3'	5.43	126.22	119.70
1	X	1003	C	O4'-C1'-N1	5.43	112.54	108.20
1	X	1626	A	P-O3'-C3'	5.43	126.21	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	413	G	C8-N9-C4	-5.43	104.23	106.40
1	X	692	C	C6-N1-C2	-5.43	118.13	120.30
1	X	1690	U	O4'-C1'-N1	5.42	112.54	108.20
2	Y	123	U	N1-C2-O2	5.42	126.60	122.80
1	X	417	C	O4'-C1'-N1	5.42	112.54	108.20
1	X	1627	C	N1-C2-O2	5.42	122.15	118.90
1	X	2039	G	N1-C2-N2	5.42	121.08	116.20
1	X	731	A	C3'-C2'-C1'	5.42	105.84	101.50
1	X	924	C	P-O3'-C3'	5.42	126.21	119.70
1	X	1753	A	C8-N9-C4	-5.42	103.63	105.80
1	X	1850	G	C8-N9-C4	-5.42	104.23	106.40
1	X	1514	C	O4'-C1'-N1	5.42	112.54	108.20
1	X	2039	G	O4'-C1'-C2'	-5.42	100.38	105.80
1	X	2405	A	N9-C1'-C2'	5.42	121.04	114.00
1	X	342	G	N7-C8-N9	5.42	115.81	113.10
19	Q	60	GLY	C-N-CA	5.42	135.24	121.70
1	X	2295	C	O4'-C1'-N1	5.41	112.53	108.20
4	B	132	LYS	C-N-CA	5.41	135.23	121.70
1	X	1380	C	O4'-C1'-N1	5.41	112.53	108.20
2	Y	88	C	P-O5'-C5'	5.41	129.56	120.90
1	X	1877	C	N1-C2-O2	5.41	122.15	118.90
1	X	2694	G	C4'-C3'-C2'	-5.41	97.19	102.60
1	X	926	C	N1-C1'-C2'	-5.41	106.05	112.00
1	X	2845	C	C6-N1-C2	-5.41	118.14	120.30
1	X	1141	U	C3'-C2'-C1'	-5.41	97.17	101.50
1	X	329	C	O4'-C1'-N1	5.41	112.53	108.20
1	X	731	A	O4'-C1'-N9	5.41	112.52	108.20
1	X	1454	U	N3-C4-C5	-5.41	111.36	114.60
1	X	2256	G	N7-C8-N9	5.41	115.80	113.10
1	X	2539	C	C6-N1-C2	-5.40	118.14	120.30
1	X	2656	G	P-O5'-C5'	-5.40	112.26	120.90
1	X	1225	G	N1-C6-O6	-5.40	116.66	119.90
1	X	1995	G	N3-C4-N9	5.40	129.24	126.00
1	X	549	G	O4'-C1'-N9	5.40	112.52	108.20
1	X	851	C	O4'-C1'-N1	5.40	112.52	108.20
1	X	1828	C	N1-C2-O2	5.40	122.14	118.90
1	X	2627	G	N1-C6-O6	5.40	123.14	119.90
2	Y	90	C	P-O5'-C5'	5.40	129.54	120.90
1	X	65	C	O4'-C1'-N1	5.39	112.52	108.20
1	X	583	C	O4'-C1'-N1	5.39	112.52	108.20
1	X	2043	A	C3'-C2'-C1'	-5.39	97.19	101.50
1	X	560	G	C4'-C3'-C2'	5.39	107.99	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	113	G	O4'-C1'-N9	5.39	112.51	108.20
1	X	1001	A	O4'-C1'-N9	5.39	112.51	108.20
1	X	1099	A	C3'-C2'-C1'	5.39	105.81	101.50
1	X	508	G	C8-N9-C4	-5.39	104.25	106.40
1	X	2335	U	O4'-C1'-N1	5.39	112.51	108.20
1	X	235	C	N1-C2-O2	5.39	122.13	118.90
1	X	647	G	O4'-C1'-N9	5.39	112.51	108.20
1	X	1255	A	O4'-C1'-N9	5.39	112.51	108.20
2	Y	45	C	O4'-C1'-N1	5.39	112.51	108.20
1	X	863	C	O4'-C1'-N1	5.38	112.51	108.20
1	X	985	G	N9-C1'-C2'	5.38	121.00	114.00
1	X	990	A	N1-C6-N6	-5.38	115.37	118.60
1	X	1632	A	N7-C8-N9	5.38	116.49	113.80
1	X	2043	A	O4'-C1'-N9	5.38	112.51	108.20
1	X	2347	C	C3'-C2'-C1'	-5.38	97.19	101.50
1	X	2659	C	O4'-C1'-N1	5.38	112.51	108.20
2	Y	44	C	N1-C2-O2	5.38	122.13	118.90
1	X	135	U	O4'-C1'-N1	5.38	112.51	108.20
1	X	2047	C	C5-C6-N1	5.38	123.69	121.00
1	X	2199	C	C5'-C4'-O4'	5.38	115.56	109.10
1	X	558	G	C8-N9-C4	-5.38	104.25	106.40
1	X	683	A	C2'-C3'-O3'	5.38	122.31	113.70
1	X	1669	A	P-O3'-C3'	5.38	126.16	119.70
1	X	1946	U	O4'-C1'-N1	5.38	112.50	108.20
1	X	2010	G	C4'-C3'-C2'	-5.38	97.22	102.60
1	X	651	C	C3'-C2'-C1'	5.38	105.80	101.50
1	X	1648	C	C5'-C4'-O4'	-5.38	102.64	109.10
1	X	306	G	P-O3'-C3'	5.38	126.16	119.70
1	X	1563	U	C5'-C4'-O4'	5.38	115.56	109.10
1	X	1979	C	O4'-C1'-N1	-5.38	103.90	108.20
1	X	2393	G	C8-N9-C4	-5.38	104.25	106.40
1	X	1825	C	C3'-C2'-C1'	-5.38	97.20	101.50
1	X	2032	G	N3-C4-N9	5.38	129.23	126.00
1	X	1694	A	O4'-C1'-N9	5.37	112.50	108.20
1	X	1811	A	C4'-C3'-C2'	5.37	107.97	102.60
1	X	2463	G	C5'-C4'-O4'	5.37	115.54	109.10
1	X	82	G	O3'-P-O5'	-5.37	93.80	104.00
1	X	1385	C	N1-C2-O2	5.37	122.12	118.90
1	X	2367	A	C5'-C4'-C3'	-5.37	107.41	116.00
1	X	2754	C	O4'-C1'-N1	5.37	112.50	108.20
1	X	1407	G	N7-C8-N9	5.37	115.78	113.10
1	X	206	U	O4'-C1'-N1	5.37	112.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	758	G	C5-C6-N1	5.37	114.18	111.50
3	A	203	ASN	CA-CB-CG	5.37	125.20	113.40
1	X	1761	G	O4'-C1'-N9	5.36	112.49	108.20
1	X	1975	G	C5-C6-N1	5.36	114.18	111.50
1	X	2703	C	C5'-C4'-O4'	5.36	115.54	109.10
1	X	655	A	C3'-C2'-C1'	5.36	105.79	101.50
1	X	934	G	O4'-C1'-N9	5.36	112.49	108.20
1	X	1018	C	O4'-C1'-N1	5.36	112.49	108.20
1	X	2004	U	P-O5'-C5'	-5.36	112.32	120.90
1	X	2299	A	P-O3'-C3'	5.36	126.13	119.70
1	X	90	G	N3-C4-C5	-5.36	125.92	128.60
1	X	560	G	C1'-O4'-C4'	5.36	114.19	109.90
1	X	1009	C	N3-C2-O2	-5.36	118.15	121.90
1	X	1069	G	C3'-C2'-C1'	5.36	105.79	101.50
1	X	405	C	N1-C2-O2	5.36	122.11	118.90
1	X	1311	C	O4'-C1'-N1	5.36	112.48	108.20
1	X	2172	U	O4'-C1'-N1	5.36	112.48	108.20
1	X	2841	U	N1-C1'-C2'	5.36	120.96	114.00
1	X	601	A	P-O5'-C5'	5.35	129.46	120.90
1	X	2067	U	O4'-C1'-N1	5.35	112.48	108.20
1	X	45	C	O4'-C1'-N1	5.35	112.48	108.20
1	X	803	C	N1-C2-O2	5.35	122.11	118.90
1	X	1637	U	O3'-P-O5'	-5.35	93.84	104.00
1	X	2069	U	O4'-C1'-N1	5.35	112.48	108.20
1	X	822	G	C8-N9-C4	-5.34	104.26	106.40
1	X	1652	G	N9-C4-C5	-5.34	103.26	105.40
1	X	2796	A	O4'-C1'-N9	5.34	112.48	108.20
1	X	2856	U	P-O3'-C3'	-5.34	113.29	119.70
1	X	2574	G	C8-N9-C4	-5.34	104.26	106.40
1	X	2631	C	N1-C2-O2	5.34	122.11	118.90
1	X	589	C	N1-C2-O2	5.34	122.11	118.90
1	X	701	U	O4'-C1'-N1	5.34	112.47	108.20
1	X	1231	A	P-O3'-C3'	-5.34	113.29	119.70
1	X	2060	A	N1-C6-N6	-5.34	115.39	118.60
1	X	2489	C	P-O5'-C5'	-5.34	112.36	120.90
1	X	1668	G	C6-C5-N7	-5.34	127.20	130.40
1	X	1673	C	O5'-P-OP1	5.34	117.10	110.70
1	X	233	A	O4'-C1'-N9	5.33	112.47	108.20
1	X	1392	U	N1-C1'-C2'	5.33	120.93	114.00
1	X	2776	U	P-O3'-C3'	5.33	126.10	119.70
1	X	2195	C	C6-N1-C2	-5.33	118.17	120.30
1	X	665	A	O4'-C1'-N9	5.33	112.46	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	11	G	O4'-C4'-C3'	-5.33	98.67	104.00
1	X	575	U	C3'-C2'-C1'	5.33	105.76	101.50
1	X	841	G	C5-N7-C8	-5.33	101.64	104.30
1	X	1341	G	N3-C4-C5	-5.33	125.94	128.60
1	X	598	U	O4'-C1'-N1	5.32	112.46	108.20
1	X	2188	A	O4'-C1'-N9	5.32	112.46	108.20
1	X	2856	U	N3-C2-O2	-5.32	118.47	122.20
1	X	1946	U	N3-C2-O2	-5.32	118.48	122.20
1	X	1060	C	O4'-C1'-N1	5.32	112.45	108.20
1	X	227	G	O4'-C1'-N9	5.32	112.45	108.20
1	X	621	U	O4'-C1'-N1	5.32	112.45	108.20
1	X	2417	U	O4'-C1'-N1	5.32	112.45	108.20
1	X	2621	G	C5'-C4'-C3'	5.32	124.51	116.00
1	X	613	A	N9-C1'-C2'	5.32	120.91	114.00
1	X	1428	G	O4'-C1'-N9	5.32	112.45	108.20
3	A	248	THR	CB-CA-C	5.32	125.95	111.60
1	X	2349	G	C3'-C2'-C1'	-5.31	97.25	101.50
1	X	1825	C	C5-C6-N1	5.31	123.66	121.00
1	X	998	C	N1-C2-O2	5.31	122.09	118.90
1	X	527	C	C4-C5-C6	-5.31	114.75	117.40
1	X	668	A	P-O3'-C3'	5.31	126.07	119.70
1	X	2419	C	N1-C2-O2	5.31	122.08	118.90
1	X	404	A	O4'-C1'-N9	5.30	112.44	108.20
1	X	63	A	C5'-C4'-C3'	-5.30	107.52	116.00
1	X	738	G	N3-C4-C5	-5.30	125.95	128.60
1	X	561	U	C5-C4-O4	-5.30	122.72	125.90
1	X	860	U	C1'-O4'-C4'	-5.30	105.66	109.90
1	X	1632	A	C8-N9-C4	-5.30	103.68	105.80
1	X	1730	G	C3'-C2'-C1'	-5.30	97.26	101.50
1	X	238	G	O4'-C1'-N9	5.30	112.44	108.20
2	Y	74	A	N7-C8-N9	5.30	116.45	113.80
1	X	1513	U	P-O3'-C3'	5.30	126.06	119.70
1	X	2377	U	O4'-C1'-N1	5.29	112.44	108.20
1	X	1358	C	P-O3'-C3'	5.29	126.05	119.70
1	X	469	G	N3-C4-C5	-5.29	125.95	128.60
1	X	1885	C	C4'-C3'-C2'	-5.29	97.31	102.60
1	X	2652	G	N3-C4-N9	5.29	129.18	126.00
1	X	327	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	646	C	C6-N1-C2	-5.29	118.19	120.30
1	X	1497	C	C5-C6-N1	5.29	123.64	121.00
1	X	723	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	2252	A	C2-N3-C4	5.29	113.24	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	145	C	O4'-C1'-N1	5.28	112.43	108.20
1	X	2867	G	C4-C5-N7	5.28	112.91	110.80
1	X	635	C	C6-N1-C2	-5.28	118.19	120.30
1	X	914	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	1008	G	C5-C6-N1	5.28	114.14	111.50
1	X	1563	U	N1-C2-O2	5.28	126.50	122.80
1	X	230	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	1398	G	P-O3'-C3'	5.28	126.03	119.70
1	X	309	G	N7-C8-N9	5.28	115.74	113.10
1	X	661	C	C6-N1-C2	-5.28	118.19	120.30
1	X	2729	A	O4'-C1'-N9	5.28	112.42	108.20
1	X	661	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	1681	A	N7-C8-N9	5.28	116.44	113.80
1	X	2426	G	P-O5'-C5'	5.28	129.34	120.90
1	X	1033	G	P-O3'-C3'	5.27	126.03	119.70
1	X	2567	G	N3-C4-C5	-5.27	125.96	128.60
2	Y	38	C	O4'-C1'-N1	5.27	112.42	108.20
1	X	1168	G	P-O5'-C5'	5.27	129.33	120.90
1	X	1742	G	P-O3'-C3'	-5.27	113.38	119.70
1	X	2004	U	O3'-P-O5'	-5.27	93.99	104.00
1	X	2026	C	O4'-C1'-N1	5.27	112.42	108.20
1	X	2525	U	O4'-C1'-N1	5.27	112.42	108.20
1	X	1238	A	P-O5'-C5'	5.27	129.33	120.90
1	X	2607	C	O4'-C1'-N1	5.27	112.42	108.20
1	X	418	C	P-O3'-C3'	5.27	126.02	119.70
1	X	1767	G	C5-C6-N1	5.27	114.13	111.50
1	X	2556	A	P-O3'-C3'	5.27	126.02	119.70
1	X	2598	C	N3-C2-O2	-5.27	118.21	121.90
1	X	327	C	C6-N1-C2	-5.27	118.19	120.30
1	X	664	C	C3'-C2'-C1'	5.26	105.71	101.50
1	X	1312	G	N7-C8-N9	5.26	115.73	113.10
1	X	1467	U	N1-C2-N3	-5.26	111.74	114.90
1	X	2628	C	O4'-C4'-C3'	-5.26	98.74	104.00
1	X	582	G	O3'-P-O5'	-5.26	94.00	104.00
1	X	1160	C	C6-N1-C2	-5.26	118.20	120.30
1	X	2463	G	P-O3'-C3'	-5.26	113.39	119.70
1	X	1142	G	C5-C6-O6	-5.26	125.44	128.60
1	X	2038	C	OP2-P-O3'	5.26	116.76	105.20
1	X	749	C	O4'-C1'-N1	5.25	112.40	108.20
1	X	850	C	O4'-C1'-N1	5.25	112.40	108.20
1	X	1252	C	O4'-C1'-N1	5.25	112.40	108.20
1	X	1235	C	C6-N1-C2	-5.25	118.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1829	C	C3'-C2'-C1'	-5.25	97.30	101.50
1	X	102	C	N1-C2-O2	5.25	122.05	118.90
1	X	203	G	O4'-C1'-N9	5.25	112.40	108.20
1	X	1150	C	P-O3'-C3'	5.25	126.00	119.70
1	X	1668	G	N1-C6-O6	5.25	123.05	119.90
1	X	2698	G	O4'-C1'-N9	5.25	112.40	108.20
2	Y	111	C	P-O3'-C3'	5.25	126.00	119.70
1	X	303	C	C5-C6-N1	5.25	123.62	121.00
1	X	429	C	C6-N1-C2	-5.25	118.20	120.30
1	X	1820	G	C4'-C3'-C2'	5.25	107.85	102.60
1	X	2225	G	C3'-C2'-C1'	-5.25	97.30	101.50
1	X	2854	G	N7-C8-N9	5.25	115.72	113.10
1	X	1288	A	N9-C1'-C2'	5.25	120.82	114.00
1	X	2667	C	C5-C6-N1	5.25	123.62	121.00
1	X	2845	C	C5-C6-N1	5.25	123.62	121.00
1	X	86	U	O4'-C1'-N1	5.24	112.39	108.20
1	X	1049	C	O4'-C1'-N1	5.24	112.39	108.20
1	X	1470	G	C8-N9-C4	-5.24	104.30	106.40
1	X	1551	U	O4'-C1'-N1	5.24	112.39	108.20
1	X	1016	C	C5-C6-N1	5.24	123.62	121.00
9	G	103	TYR	C-N-CA	5.24	134.80	121.70
1	X	186	C	N1-C2-O2	5.24	122.04	118.90
1	X	488	A	O4'-C1'-N9	5.24	112.39	108.20
1	X	846	A	O4'-C1'-N9	5.24	112.39	108.20
1	X	1977	C	O4'-C1'-N1	5.24	112.39	108.20
2	Y	29	C	C6-N1-C2	-5.24	118.20	120.30
1	X	1083	C	O4'-C1'-N1	5.24	112.39	108.20
1	X	1683	G	N9-C1'-C2'	-5.24	106.24	112.00
1	X	1355	A	O4'-C1'-N9	5.24	112.39	108.20
1	X	2035	G	C8-N9-C4	-5.24	104.31	106.40
1	X	2165	A	P-O3'-C3'	5.24	125.98	119.70
1	X	2321	C	N1-C2-O2	5.24	122.04	118.90
1	X	2330	G	N3-C4-C5	-5.24	125.98	128.60
1	X	2340	C	C6-N1-C2	-5.24	118.21	120.30
1	X	683	A	O4'-C1'-N9	-5.23	104.01	108.20
1	X	1312	G	C8-N9-C4	-5.23	104.31	106.40
1	X	2602	G	N3-C4-C5	-5.23	125.98	128.60
1	X	70	A	C3'-C2'-C1'	5.23	105.69	101.50
1	X	104	C	O4'-C1'-N1	5.23	112.38	108.20
1	X	572	G	C5-C6-N1	5.23	114.11	111.50
1	X	582	G	C3'-C2'-C1'	5.23	105.68	101.50
1	X	2535	C	N1-C2-O2	5.23	122.04	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	227	G	N9-C1'-C2'	5.23	120.80	114.00
1	X	1573	G	P-O3'-C3'	5.23	125.97	119.70
1	X	2246	A	C2-N3-C4	5.23	113.21	110.60
1	X	2626	U	N3-C2-O2	-5.23	118.54	122.20
1	X	148	C	O4'-C1'-N1	5.23	112.38	108.20
1	X	1563	U	N3-C2-O2	-5.23	118.54	122.20
1	X	788	G	O4'-C1'-N9	5.22	112.38	108.20
1	X	1150	C	N1-C2-O2	5.22	122.03	118.90
1	X	2326	C	C6-N1-C2	-5.22	118.21	120.30
1	X	2432	A	C8-N9-C4	-5.22	103.71	105.80
1	X	2805	G	C8-N9-C4	-5.22	104.31	106.40
1	X	312	G	O4'-C1'-N9	5.22	112.38	108.20
1	X	1663	C	O4'-C1'-N1	5.22	112.38	108.20
1	X	2075	U	C1'-O4'-C4'	-5.22	105.72	109.90
1	X	2602	G	C5-C6-N1	5.22	114.11	111.50
1	X	689	A	C2-N3-C4	-5.22	107.99	110.60
1	X	782	U	O4'-C1'-N1	5.22	112.38	108.20
1	X	878	C	P-O3'-C3'	5.22	125.96	119.70
1	X	1284	G	C6-C5-N7	-5.22	127.27	130.40
1	X	2632	U	O4'-C1'-N1	5.22	112.38	108.20
1	X	2696	A	C4'-C3'-C2'	-5.22	97.38	102.60
1	X	349	G	P-O5'-C5'	5.21	129.24	120.90
1	X	1624	A	P-O3'-C3'	5.21	125.95	119.70
1	X	1663	C	O3'-P-O5'	-5.21	94.09	104.00
1	X	352	G	O4'-C1'-N9	5.21	112.37	108.20
1	X	413	G	N7-C8-N9	5.21	115.71	113.10
1	X	2550	C	P-O3'-C3'	5.21	125.95	119.70
1	X	2794	G	O5'-P-OP2	-5.21	101.01	105.70
1	X	1312	G	C6-C5-N7	-5.21	127.27	130.40
1	X	313	U	O4'-C1'-N1	5.21	112.37	108.20
1	X	2715	C	P-O5'-C5'	5.21	129.24	120.90
1	X	2843	A	C5'-C4'-C3'	-5.21	107.67	116.00
17	O	6	GLN	C-N-CA	5.21	134.72	121.70
1	X	475	U	N3-C2-O2	-5.21	118.56	122.20
1	X	967	G	O4'-C1'-N9	5.21	112.37	108.20
1	X	1064	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	1271	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	1549	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	1824	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	1284	G	C8-N9-C4	-5.21	104.32	106.40
1	X	1344	C	N1-C2-O2	5.21	122.02	118.90
1	X	2511	G	P-O5'-C5'	5.21	129.23	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2033	C	N3-C2-O2	-5.20	118.26	121.90
1	X	2326	C	P-O3'-C3'	-5.20	113.46	119.70
1	X	2671	C	P-O5'-C5'	-5.20	112.58	120.90
1	X	76	C	N1-C2-O2	5.20	122.02	118.90
1	X	1435	G	C8-N9-C4	-5.20	104.32	106.40
1	X	20	C	O4'-C1'-N1	5.20	112.36	108.20
1	X	507	A	P-O3'-C3'	-5.20	113.46	119.70
1	X	1327	C	C6-N1-C2	-5.20	118.22	120.30
1	X	1764	A	C2'-C3'-O3'	5.20	122.02	113.70
1	X	2318	U	O4'-C1'-N1	5.20	112.36	108.20
1	X	2560	G	N9-C4-C5	5.20	107.48	105.40
1	X	540	G	C4-C5-N7	-5.20	108.72	110.80
1	X	722	C	N1-C2-O2	5.20	122.02	118.90
1	X	2406	C	O4'-C1'-N1	5.19	112.36	108.20
1	X	168	A	OP1-P-O3'	5.19	116.62	105.20
1	X	1276	U	P-O3'-C3'	5.19	125.93	119.70
3	A	243	GLY	C-N-CA	5.19	134.68	121.70
1	X	682	G	C1'-O4'-C4'	-5.19	105.75	109.90
1	X	1105	U	O4'-C1'-N1	5.19	112.35	108.20
1	X	1466	C	C2-N1-C1'	5.19	124.51	118.80
1	X	2463	G	N3-C4-C5	-5.19	126.00	128.60
1	X	831	G	C8-N9-C4	-5.19	104.33	106.40
1	X	1312	G	P-O3'-C3'	5.19	125.92	119.70
1	X	2825	A	N1-C6-N6	5.19	121.71	118.60
11	I	38	LYS	C-N-CA	5.19	134.66	121.70
1	X	2537	C	O4'-C1'-N1	5.18	112.35	108.20
1	X	34	U	P-O5'-C5'	5.18	129.19	120.90
1	X	1652	G	N1-C6-O6	5.18	123.01	119.90
1	X	430	C	C5-C6-N1	5.18	123.59	121.00
1	X	883	A	O4'-C1'-N9	5.18	112.34	108.20
2	Y	23	G	O4'-C1'-N9	5.18	112.34	108.20
1	X	1223	G	N7-C8-N9	5.18	115.69	113.10
1	X	1935	A	C2-N3-C4	5.18	113.19	110.60
1	X	7	G	C8-N9-C4	-5.18	104.33	106.40
1	X	795	A	P-O3'-C3'	5.18	125.91	119.70
1	X	2018	G	N7-C8-N9	5.18	115.69	113.10
1	X	465	C	C1'-O4'-C4'	-5.17	105.76	109.90
1	X	624	A	C2-N3-C4	5.17	113.19	110.60
1	X	951	G	C3'-C2'-C1'	-5.17	97.36	101.50
1	X	1466	C	O4'-C1'-N1	5.17	112.34	108.20
1	X	174	A	P-O5'-C5'	5.17	129.17	120.90
1	X	597	U	C5-C4-O4	-5.17	122.80	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	765	C	N1-C2-O2	5.17	122.00	118.90
1	X	1530	U	O4'-C1'-N1	5.17	112.34	108.20
1	X	1824	C	N3-C2-O2	-5.17	118.28	121.90
1	X	2420	C	P-O5'-C5'	5.17	129.17	120.90
1	X	516	G	C4-C5-N7	5.17	112.87	110.80
1	X	652	C	C5'-C4'-C3'	-5.17	107.73	116.00
1	X	1488	G	O4'-C1'-N9	5.17	112.33	108.20
1	X	2326	C	C5-C6-N1	5.17	123.58	121.00
2	Y	92	G	C5'-C4'-O4'	5.17	115.30	109.10
1	X	7	G	C5'-C4'-C3'	-5.17	107.73	116.00
1	X	2503	G	C5-C6-O6	-5.17	125.50	128.60
1	X	956	A	O3'-P-O5'	-5.17	94.19	104.00
1	X	2854	G	C8-N9-C4	-5.17	104.33	106.40
1	X	462	G	C5-C6-N1	-5.16	108.92	111.50
1	X	540	G	N3-C4-C5	-5.16	126.02	128.60
1	X	582	G	C2-N3-C4	5.16	114.48	111.90
1	X	1000	G	O4'-C1'-C2'	-5.16	100.64	105.80
1	X	1623	C	N1-C2-O2	5.16	122.00	118.90
2	Y	14	C	C3'-C2'-C1'	5.16	105.63	101.50
1	X	545	C	O4'-C1'-N1	5.16	112.33	108.20
1	X	1426	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2626	U	N1-C2-O2	5.16	126.41	122.80
1	X	207	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	648	A	P-O3'-C3'	5.16	125.89	119.70
1	X	1790	G	N9-C1'-C2'	5.16	120.71	114.00
1	X	2793	G	O4'-C1'-N9	5.16	112.33	108.20
1	X	780	U	O4'-C1'-N1	5.16	112.32	108.20
1	X	1010	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	811	G	P-O3'-C3'	-5.15	113.52	119.70
2	Y	45	C	N3-C2-O2	-5.15	118.29	121.90
2	Y	102	A	O4'-C1'-N9	5.15	112.32	108.20
1	X	2170	C	O4'-C1'-N1	5.15	112.32	108.20
1	X	2825	A	P-O3'-C3'	5.15	125.88	119.70
11	I	28	LYS	C-N-CA	5.15	134.57	121.70
1	X	2776	U	O4'-C1'-N1	5.15	112.32	108.20
1	X	439	C	O4'-C1'-N1	5.15	112.32	108.20
1	X	1138	A	P-O5'-C5'	5.15	129.13	120.90
1	X	1668	G	P-O3'-C3'	-5.15	113.53	119.70
1	X	818	G	N7-C8-N9	5.14	115.67	113.10
1	X	998	C	C5'-C4'-C3'	5.14	124.23	116.00
1	X	2264	C	P-O3'-C3'	-5.14	113.53	119.70
1	X	2478	C	C5-C6-N1	5.14	123.57	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	178	C	O4'-C1'-N1	5.14	112.31	108.20
1	X	2034	A	C5-C6-N6	-5.14	119.58	123.70
1	X	1236	G	O4'-C1'-N9	5.14	112.31	108.20
1	X	2654	A	C2-N3-C4	5.14	113.17	110.60
1	X	1714	A	O4'-C1'-N9	5.14	112.31	108.20
1	X	607	C	N3-C2-O2	-5.14	118.31	121.90
1	X	1097	A	P-O3'-C3'	5.14	125.86	119.70
1	X	2028	C	O4'-C4'-C3'	-5.14	98.86	104.00
1	X	2537	C	P-O3'-C3'	-5.14	113.54	119.70
1	X	2658	A	O4'-C1'-N9	5.14	112.31	108.20
1	X	2824	C	C2'-C3'-O3'	5.14	121.92	113.70
1	X	1930	C	N1-C2-O2	5.13	121.98	118.90
1	X	1396	C	C5-C6-N1	5.13	123.57	121.00
1	X	1219	C	O4'-C1'-N1	5.13	112.31	108.20
1	X	1268	U	P-O5'-C5'	5.13	129.11	120.90
1	X	1744	G	C6-N1-C2	-5.13	122.02	125.10
1	X	2555	G	C5-C6-N1	5.13	114.07	111.50
1	X	2828	C	O4'-C1'-N1	5.13	112.30	108.20
1	X	519	C	O4'-C1'-N1	5.13	112.30	108.20
1	X	1142	G	C5-C6-N1	5.13	114.06	111.50
1	X	1345	G	P-O3'-C3'	5.13	125.86	119.70
1	X	1876	C	N1-C2-O2	5.13	121.98	118.90
1	X	2381	A	O4'-C1'-N9	5.13	112.30	108.20
1	X	540	G	C3'-C2'-C1'	5.13	105.60	101.50
1	X	1946	U	N1-C2-O2	5.13	126.39	122.80
1	X	1681	A	C8-N9-C4	-5.12	103.75	105.80
1	X	170	U	N1-C2-O2	5.12	126.39	122.80
1	X	27	G	O4'-C1'-N9	5.12	112.30	108.20
1	X	1403	U	C3'-C2'-C1'	5.12	105.60	101.50
1	X	2229	G	C2-N3-C4	5.12	114.46	111.90
1	X	1106	A	P-O3'-C3'	5.12	125.84	119.70
1	X	2688	G	C5-C6-O6	-5.12	125.53	128.60
2	Y	67	C	P-O3'-C3'	5.12	125.84	119.70
1	X	1123	G	P-O3'-C3'	5.12	125.84	119.70
1	X	1142	G	C6-N1-C2	-5.12	122.03	125.10
1	X	2016	A	P-O3'-C3'	5.12	125.84	119.70
1	X	1407	G	C6-C5-N7	-5.12	127.33	130.40
1	X	1607	A	C3'-C2'-C1'	-5.12	97.41	101.50
1	X	1725	C	P-O5'-C5'	-5.12	112.71	120.90
1	X	2615	U	O4'-C1'-N1	5.12	112.29	108.20
2	Y	90	C	C4'-C3'-O3'	5.12	123.23	113.00
1	X	2660	C	P-O5'-C5'	5.11	129.08	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2748	C	N1-C1'-C2'	-5.11	106.37	112.00
1	X	596	C	P-O5'-C5'	-5.11	112.72	120.90
1	X	2660	C	P-O3'-C3'	5.11	125.83	119.70
1	X	499	G	C5-C6-N1	5.11	114.06	111.50
1	X	552	C	N1-C2-O2	5.11	121.97	118.90
1	X	934	G	N7-C8-N9	5.11	115.66	113.10
1	X	1666	G	C5-C6-N1	5.11	114.06	111.50
1	X	2369	U	O4'-C1'-N1	5.11	112.29	108.20
1	X	2606	G	C5'-C4'-O4'	5.11	115.23	109.10
1	X	236	C	C5-C6-N1	5.11	123.55	121.00
1	X	247	A	C5'-C4'-O4'	5.11	115.23	109.10
1	X	1337	G	P-O5'-C5'	5.11	129.07	120.90
1	X	1540	C	O4'-C1'-N1	5.11	112.28	108.20
1	X	1663	C	C2-N1-C1'	5.10	124.41	118.80
1	X	2667	C	P-O3'-C3'	5.10	125.82	119.70
1	X	1010	U	P-O5'-C5'	5.10	129.06	120.90
1	X	1097	A	O4'-C1'-N9	5.10	112.28	108.20
1	X	2032	G	C5-C6-N1	5.10	114.05	111.50
1	X	480	G	C3'-C2'-C1'	-5.10	97.42	101.50
1	X	688	A	P-O3'-C3'	5.10	125.82	119.70
1	X	333	A	O4'-C1'-N9	5.10	112.28	108.20
1	X	854	G	C3'-C2'-C1'	-5.10	97.42	101.50
1	X	2526	U	O4'-C1'-N1	5.10	112.28	108.20
1	X	2826	C	N1-C2-O2	5.10	121.96	118.90
2	Y	19	C	N3-C2-O2	-5.10	118.33	121.90
1	X	402	A	P-O3'-C3'	-5.09	113.59	119.70
1	X	459	A	C2-N3-C4	5.09	113.15	110.60
1	X	616	U	O4'-C1'-N1	5.09	112.28	108.20
1	X	996	C	N3-C2-O2	-5.09	118.33	121.90
1	X	1254	G	N3-C4-C5	-5.09	126.05	128.60
1	X	1337	G	O5'-P-OP2	-5.09	101.11	105.70
1	X	98	U	N3-C2-O2	-5.09	118.64	122.20
1	X	542	A	N7-C8-N9	5.09	116.35	113.80
1	X	1198	C	O4'-C1'-N1	5.09	112.27	108.20
1	X	1648	C	N1-C2-O2	5.09	121.95	118.90
1	X	1870	U	O4'-C1'-N1	5.09	112.27	108.20
1	X	2774	U	P-O3'-C3'	5.09	125.81	119.70
1	X	2195	C	O4'-C1'-N1	5.08	112.27	108.20
1	X	2702	G	O4'-C1'-N9	-5.08	104.13	108.20
1	X	179	U	O4'-C1'-N1	5.08	112.27	108.20
1	X	540	G	C2-N3-C4	5.08	114.44	111.90
1	X	757	U	OP2-P-O3'	5.08	116.39	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2015	G	C5-N7-C8	-5.08	101.76	104.30
2	Y	100	G	O4'-C1'-N9	5.08	112.27	108.20
1	X	1015	U	O4'-C1'-N1	5.08	112.27	108.20
1	X	1321	A	C3'-C2'-C1'	-5.08	97.43	101.50
1	X	1801	C	N1-C2-O2	5.08	121.95	118.90
2	Y	53	G	O4'-C1'-N9	5.08	112.26	108.20
1	X	1497	C	O4'-C1'-N1	5.08	112.26	108.20
1	X	516	G	O4'-C1'-N9	5.08	112.26	108.20
1	X	625	A	P-O3'-C3'	5.08	125.79	119.70
1	X	1248	G	O4'-C1'-N9	-5.08	104.14	108.20
1	X	1266	G	P-O3'-C3'	5.07	125.79	119.70
1	X	1882	G	C8-N9-C4	-5.07	104.37	106.40
1	X	2727	G	O4'-C1'-N9	5.07	112.26	108.20
2	Y	94	G	C5'-C4'-O4'	5.07	115.19	109.10
1	X	227	G	C8-N9-C4	-5.07	104.37	106.40
1	X	1863	U	O4'-C1'-N1	5.07	112.26	108.20
1	X	985	G	C5-C6-N1	5.07	114.03	111.50
1	X	1384	G	P-O3'-C3'	5.07	125.78	119.70
1	X	2848	A	O4'-C1'-N9	5.07	112.26	108.20
1	X	2588	U	C5'-C4'-O4'	5.07	115.18	109.10
1	X	358	C	P-O5'-C5'	5.07	129.01	120.90
1	X	807	A	O4'-C1'-N9	5.07	112.25	108.20
1	X	934	G	C8-N9-C4	-5.07	104.37	106.40
1	X	1766	U	P-O3'-C3'	5.07	125.78	119.70
1	X	1922	U	N3-C2-O2	-5.07	118.65	122.20
1	X	2261	G	C4'-C3'-C2'	5.07	107.67	102.60
1	X	2452	U	N3-C2-O2	-5.07	118.65	122.20
1	X	16	G	N3-C4-N9	5.06	129.04	126.00
2	Y	123	U	C6-N1-C1'	-5.06	114.11	121.20
1	X	22	C	P-O3'-C3'	5.06	125.78	119.70
1	X	1037	U	C1'-O4'-C4'	-5.06	105.85	109.90
1	X	1625	A	P-O3'-C3'	5.06	125.78	119.70
1	X	1690	U	P-O5'-C5'	-5.06	112.80	120.90
1	X	2000	U	N3-C4-O4	5.06	122.94	119.40
1	X	2264	C	C3'-C2'-C1'	-5.06	97.45	101.50
1	X	2442	C	N1-C2-O2	5.06	121.94	118.90
1	X	2213	G	C8-N9-C4	-5.06	104.38	106.40
1	X	2718	A	C5'-C4'-O4'	5.06	115.17	109.10
1	X	93	A	O4'-C1'-N9	5.06	112.25	108.20
1	X	569	C	O4'-C1'-N1	5.06	112.25	108.20
1	X	2568	A	O4'-C4'-C3'	-5.06	98.94	104.00
1	X	672	C	C3'-C2'-C1'	-5.06	97.45	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2210	C	O4'-C1'-N1	5.06	112.25	108.20
1	X	1152	C	P-O5'-C5'	5.06	128.99	120.90
1	X	940	G	C8-N9-C4	-5.05	104.38	106.40
1	X	1608	U	P-O3'-C3'	5.05	125.77	119.70
1	X	1971	C	P-O5'-C5'	-5.05	112.81	120.90
1	X	2314	A	O4'-C1'-N9	5.05	112.24	108.20
2	Y	86	A	C5'-C4'-O4'	5.05	115.17	109.10
1	X	1965	U	C5'-C4'-C3'	-5.05	107.92	116.00
1	X	2592	U	C5'-C4'-O4'	5.05	115.16	109.10
1	X	2824	C	N1-C1'-C2'	5.05	120.57	114.00
1	X	354	C	O4'-C1'-N1	5.05	112.24	108.20
1	X	1383	C	O4'-C1'-N1	5.05	112.24	108.20
1	X	1481	U	O4'-C1'-N1	5.05	112.24	108.20
1	X	1975	G	C3'-C2'-C1'	5.05	105.54	101.50
1	X	184	A	N1-C6-N6	-5.05	115.57	118.60
1	X	998	C	C4'-C3'-C2'	-5.05	97.55	102.60
1	X	860	U	C2-N1-C1'	5.05	123.75	117.70
1	X	2468	G	C2-N3-C4	5.05	114.42	111.90
1	X	869	C	C6-N1-C2	-5.04	118.28	120.30
1	X	916	U	O4'-C1'-N1	5.04	112.23	108.20
1	X	940	G	P-O3'-C3'	5.04	125.75	119.70
1	X	1132	C	C5-C6-N1	5.04	123.52	121.00
1	X	1619	A	P-O3'-C3'	5.04	125.75	119.70
1	X	2527	G	P-O5'-C5'	-5.04	112.83	120.90
1	X	42	G	O4'-C1'-N9	5.04	112.23	108.20
1	X	332	C	C1'-O4'-C4'	-5.04	105.87	109.90
1	X	570	G	P-O3'-C3'	5.04	125.75	119.70
1	X	598	U	O4'-C4'-C3'	-5.04	98.96	104.00
1	X	1219	C	C6-N1-C2	-5.04	118.28	120.30
1	X	1337	G	C4'-C3'-C2'	5.04	107.64	102.60
1	X	1909	U	P-O3'-C3'	5.04	125.75	119.70
1	X	1496	G	C4'-C3'-O3'	5.04	123.08	113.00
1	X	670	U	N1-C2-O2	5.04	126.33	122.80
1	X	1162	A	C4'-C3'-C2'	-5.04	97.56	102.60
1	X	2620	G	P-O3'-C3'	5.04	125.75	119.70
1	X	1825	C	C6-N1-C2	-5.04	118.28	120.30
1	X	1881	U	O4'-C1'-N1	5.04	112.23	108.20
1	X	1973	C	O4'-C1'-N1	5.04	112.23	108.20
1	X	1470	G	C5-C6-O6	-5.04	125.58	128.60
1	X	1689	U	N3-C2-O2	-5.04	118.68	122.20
1	X	2311	U	O4'-C1'-N1	5.04	112.23	108.20
1	X	2702	G	C5-N7-C8	-5.04	101.78	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2831	A	C2-N3-C4	5.04	113.12	110.60
3	A	203	ASN	CB-CA-C	5.04	120.47	110.40
1	X	615	C	O4'-C1'-N1	5.03	112.23	108.20
1	X	689	A	C4-C5-N7	5.03	113.22	110.70
1	X	2527	G	N3-C4-C5	-5.03	126.08	128.60
2	Y	119	G	O4'-C1'-N9	5.03	112.23	108.20
1	X	684	C	C4-C5-C6	5.03	119.92	117.40
1	X	2340	C	O4'-C1'-N1	5.03	112.23	108.20
1	X	303	C	O4'-C1'-N1	5.03	112.22	108.20
1	X	636	G	C5'-C4'-C3'	-5.03	107.95	116.00
1	X	2038	C	P-O3'-C3'	5.03	125.74	119.70
1	X	2340	C	C5-C6-N1	5.03	123.52	121.00
1	X	1663	C	C3'-C2'-C1'	5.03	105.52	101.50
1	X	11	G	N7-C8-N9	5.03	115.61	113.10
1	X	311	A	O4'-C1'-N9	5.03	112.22	108.20
1	X	1010	U	N3-C2-O2	-5.03	118.68	122.20
1	X	1122	A	O4'-C1'-N9	5.03	112.22	108.20
1	X	1570	C	O4'-C1'-N1	5.03	112.22	108.20
1	X	2015	G	C5-C6-N1	5.03	114.01	111.50
1	X	2635	U	N3-C2-O2	-5.03	118.68	122.20
1	X	2780	A	P-O5'-C5'	5.03	128.94	120.90
1	X	518	A	P-O5'-C5'	5.02	128.94	120.90
1	X	1731	C	C3'-C2'-C1'	-5.02	97.48	101.50
1	X	2062	U	O4'-C1'-N1	5.02	112.22	108.20
2	Y	77	G	P-O5'-C5'	5.02	128.94	120.90
1	X	2254	C	N1-C2-O2	5.02	121.91	118.90
1	X	2740	C	N1-C2-O2	5.02	121.91	118.90
1	X	677	G	O4'-C1'-N9	5.02	112.22	108.20
1	X	2582	G	C6-C5-N7	-5.02	127.39	130.40
1	X	622	U	O4'-C1'-N1	5.02	112.22	108.20
1	X	661	C	N3-C2-O2	-5.02	118.39	121.90
1	X	978	U	O4'-C1'-N1	5.02	112.22	108.20
1	X	834	A	P-O3'-C3'	-5.02	113.68	119.70
1	X	1128	G	P-O5'-C5'	5.02	128.93	120.90
1	X	1679	U	N3-C2-O2	-5.02	118.69	122.20
1	X	2619	G	N1-C6-O6	5.02	122.91	119.90
1	X	416	U	C1'-O4'-C4'	-5.02	105.89	109.90
1	X	863	C	C6-N1-C2	-5.02	118.29	120.30
1	X	1785	A	P-O5'-C5'	-5.02	112.87	120.90
1	X	1429	A	O4'-C1'-N9	5.01	112.21	108.20
1	X	1603	A	P-O3'-C3'	5.01	125.72	119.70
1	X	534	U	P-O5'-C5'	5.01	128.92	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	941	U	C4'-C3'-C2'	-5.01	97.59	102.60
1	X	1661	C	N1-C2-O2	5.01	121.91	118.90
1	X	1932	G	O4'-C1'-N9	5.01	112.21	108.20
1	X	216	U	N3-C2-O2	-5.01	118.69	122.20
1	X	1533	G	N7-C8-N9	5.01	115.60	113.10
1	X	1886	G	C8-N9-C4	-5.01	104.40	106.40
2	Y	12	C	O4'-C1'-N1	5.01	112.21	108.20
1	X	19	C	P-O3'-C3'	-5.01	113.69	119.70
1	X	581	A	O3'-P-O5'	-5.01	94.49	104.00
1	X	1652	G	N3-C4-N9	5.01	129.00	126.00
1	X	349	G	O4'-C1'-N9	5.00	112.20	108.20
1	X	631	G	C1'-O4'-C4'	-5.00	105.90	109.90
1	X	2487	G	C8-N9-C4	-5.00	104.40	106.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1251	G	Sidechain
1	X	699	G	Sidechain
1	X	967	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29049	535	0
2	Y	2598	0	1328	22	0
3	A	1826	0	1885	83	0
4	B	1539	0	1600	57	0
5	C	1506	0	1525	57	0
6	D	1400	0	1481	17	0
7	E	1286	0	1336	10	0
8	F	503	0	520	5	0
9	G	1114	0	1144	46	0
10	H	997	0	1046	30	0
11	I	1067	0	1103	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	J	1090	0	1125	31	0
13	K	878	0	930	24	0
14	L	779	0	820	19	0
15	M	871	0	894	25	0
16	N	978	0	1020	33	0
17	O	741	0	756	24	0
18	P	1014	0	1096	23	0
19	Q	726	0	753	11	0
20	R	825	0	881	26	0
21	S	1345	0	1372	30	0
22	T	625	0	655	11	0
23	U	552	0	604	31	0
24	V	533	0	558	7	0
25	W	424	0	470	15	0
26	Z	457	0	462	20	0
27	1	53	0	0	0	0
28	2	46	0	0	1	0
29	3	63	0	0	0	0
30	4	297	0	330	4	0
31	M	1	0	0	0	0
31	X	28	0	0	0	0
31	Y	6	0	0	0	0
32	X	58	0	67	19	0
All	All	83877	0	54810	1080	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1080) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:117:MET:SD	4:B:117:MET:CE	2.02	1.47
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.69	1.08
9:G:33:ILE:HB	9:G:34:PRO:HD3	1.38	1.03
1:X:558:G:H4'	1:X:559:C:H5'	1.40	1.02
1:X:1448:A:H61	1:X:1574:A:H61	1.09	1.00
5:C:43:ALA:HB1	5:C:86:PRO:HB2	1.46	0.96
4:B:152:LYS:HB2	9:G:106:TYR:HB3	1.49	0.95
1:X:1542:G:H22	1:X:1562:G:H1	1.13	0.94
1:X:1007:A:H4'	16:N:93:LYS:HB3	1.46	0.94
1:X:1919:A:H2	1:X:1926:U:H3	1.09	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:116:VAL:HG22	4:B:136:ARG:HE	1.31	0.93
11:I:62:LYS:HE2	11:I:64:GLY:HA3	1.53	0.91
32:X:2929:1F4:H59	32:X:2929:1F4:H60	1.51	0.90
11:I:30:ALA:HB3	11:I:34:HIS:CE1	2.07	0.89
15:M:79:ARG:HH11	15:M:79:ARG:HG3	1.36	0.88
1:X:77:C:H42	1:X:106:G:H1	1.21	0.88
1:X:1770:U:H5	1:X:1775:A:N7	1.70	0.88
14:L:38:ILE:HG13	14:L:39:TYR:H	1.39	0.88
4:B:116:VAL:HG22	4:B:136:ARG:NE	1.88	0.87
21:S:71:MET:HA	21:S:78:PRO:HA	1.58	0.85
4:B:131:SER:HB3	4:B:134:TRP:CD1	2.11	0.85
3:A:252:LYS:HD2	3:A:253:PRO:HD3	1.59	0.84
1:X:1817:U:H4'	3:A:252:LYS:HE2	1.59	0.83
1:X:1266:G:N7	11:I:32:ARG:NH1	2.25	0.83
13:K:10:LEU:HD21	13:K:17:ARG:HB2	1.61	0.82
3:A:248:THR:HB	3:A:249:PRO:HD3	1.60	0.82
1:X:2371:A:H2	1:X:2403:C:H42	1.28	0.82
3:A:218:LYS:HE3	3:A:221:GLN:HB2	1.62	0.82
1:X:38:G:H1	1:X:453:U:H3	1.25	0.81
1:X:1278:A:H2	1:X:1997:A:H62	1.26	0.80
9:G:33:ILE:HB	9:G:34:PRO:CD	2.11	0.80
1:X:2387:U:H2'	1:X:2388:G:H8	1.45	0.80
9:G:100:TYR:HB2	9:G:116:ARG:HH11	1.47	0.79
1:X:1342:U:H5''	1:X:1343:C:H5	1.48	0.78
3:A:43:ARG:N	3:A:43:ARG:HD2	1.99	0.78
1:X:559:C:H2'	1:X:560:G:O4'	1.84	0.78
9:G:68:PRO:HD2	9:G:76:GLN:HB3	1.66	0.78
1:X:823:U:OP1	11:I:32:ARG:NH1	2.17	0.78
32:X:2929:1F4:H3	32:X:2929:1F4:C39	2.13	0.78
16:N:66:ASN:HB3	16:N:76:TYR:H	1.50	0.77
1:X:640:C:H4'	1:X:660:G:H21	1.49	0.77
15:M:59:GLY:HA3	15:M:64:LYS:HA	1.65	0.77
3:A:172:TYR:HA	3:A:186:HIS:HA	1.66	0.76
1:X:224:G:OP2	1:X:226:C:N4	2.17	0.76
5:C:29:GLU:HB2	11:I:18:ARG:HH12	1.50	0.76
1:X:673:G:H5'	5:C:93:TYR:CE1	2.20	0.76
14:L:33:ARG:HD2	14:L:38:ILE:HD13	1.66	0.76
1:X:689:A:H8	1:X:2052:G:H21	1.33	0.76
26:Z:35:GLN:O	26:Z:37:HIS:N	2.19	0.76
21:S:6:LYS:H	21:S:7:PRO:HD3	1.48	0.75
1:X:1007:A:H1'	17:O:6:GLN:HG2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:4:HIS:HB3	26:Z:5:PRO:HD3	1.69	0.75
13:K:10:LEU:CD2	13:K:17:ARG:HB2	2.15	0.75
4:B:134:TRP:H	4:B:134:TRP:HD1	1.32	0.75
2:Y:45:C:H2'	6:D:92:ARG:HH11	1.52	0.75
15:M:79:ARG:HH11	15:M:79:ARG:CG	2.00	0.75
10:H:25:LEU:HD11	10:H:52:VAL:HG23	1.70	0.73
25:W:12:ARG:HH11	25:W:12:ARG:HG2	1.52	0.73
1:X:1329:U:H2'	1:X:1330:G:H8	1.52	0.73
1:X:1919:A:H2	1:X:1926:U:N3	1.84	0.73
17:O:73:LYS:HB2	17:O:82:ARG:HB2	1.70	0.73
1:X:652:C:H42	1:X:657:A:H61	1.35	0.73
15:M:79:ARG:HG3	15:M:79:ARG:NH1	2.02	0.73
9:G:100:TYR:HB2	9:G:116:ARG:HH12	1.51	0.72
17:O:57:GLN:H	17:O:97:GLY:HA3	1.53	0.72
1:X:2387:U:H2'	1:X:2388:G:C8	2.23	0.72
11:I:62:LYS:CE	11:I:64:GLY:HA3	2.19	0.72
1:X:1329:U:H2'	1:X:1330:G:C8	2.25	0.72
4:B:152:LYS:CB	9:G:106:TYR:HB3	2.20	0.71
5:C:48:ARG:HB2	5:C:51:VAL:HG22	1.70	0.71
11:I:62:LYS:HE2	11:I:64:GLY:CA	2.20	0.71
1:X:2241:U:H5	22:T:17:ASN:OD1	1.72	0.71
1:X:617:U:H5	1:X:632:A:H2	1.38	0.70
3:A:231:HIS:HD2	3:A:233:HIS:H	1.38	0.70
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.73	0.70
1:X:617:U:C5	1:X:632:A:C2	2.80	0.70
3:A:243:GLY:C	3:A:244:ARG:HD3	2.11	0.70
1:X:1673:C:H2'	1:X:1674:C:H6	1.55	0.70
4:B:110:GLY:O	13:K:3:HIS:CD2	2.45	0.70
1:X:2039:G:N2	26:Z:4:HIS:O	2.22	0.69
4:B:14:ILE:HG22	4:B:21:ILE:HB	1.74	0.69
13:K:79:VAL:HA	13:K:83:VAL:HG13	1.73	0.69
1:X:1561:A:H3'	1:X:1562:G:C8	2.27	0.69
23:U:48:LYS:CG	23:U:49:LYS:H	2.04	0.69
1:X:1832:G:H1	1:X:1885:C:H42	1.37	0.69
1:X:2063:A:H4'	23:U:39:LYS:HG2	1.73	0.69
3:A:231:HIS:CD2	3:A:233:HIS:H	2.11	0.69
14:L:33:ARG:NH1	14:L:38:ILE:HB	2.08	0.68
1:X:1466:C:H2'	1:X:1467:U:O4'	1.93	0.68
1:X:1278:A:N6	1:X:1996:A:H5''	2.08	0.68
1:X:501:G:H2'	1:X:502:A:C8	2.28	0.68
1:X:577:U:H2'	1:X:579:G:OP2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:61:ARG:NH1	9:G:66:HIS:H	1.90	0.67
1:X:2770:A:H4'	1:X:2771:C:H5'	1.74	0.67
1:X:1882:G:N2	1:X:1885:C:H41	1.92	0.67
1:X:1278:A:H61	1:X:1996:A:H5''	1.60	0.67
1:X:2767:C:H1'	4:B:62:PRO:HG3	1.77	0.67
25:W:12:ARG:CG	25:W:12:ARG:HH11	2.06	0.67
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.76	0.67
9:G:132:PHE:CZ	9:G:145:HIS:HB2	2.30	0.67
9:G:67:ARG:HG2	9:G:70:PHE:HA	1.76	0.67
13:K:11:ASN:OD1	13:K:17:ARG:NH2	2.27	0.67
3:A:43:ARG:HE	3:A:55:GLY:HA2	1.60	0.67
9:G:104:THR:OG1	9:G:110:LEU:HB3	1.95	0.67
20:R:7:GLY:HA3	20:R:42:ARG:O	1.94	0.67
1:X:1885:C:C4'	3:A:244:ARG:HD2	2.24	0.66
1:X:168:A:H2'	1:X:169:C:C6	2.30	0.66
1:X:341:A:HO2'	1:X:342:G:H8	1.41	0.66
1:X:1342:U:H5''	1:X:1343:C:C5	2.31	0.66
32:X:2929:1F4:H3	32:X:2929:1F4:H51	1.76	0.66
32:X:2929:1F4:C50	32:X:2929:1F4:H60	2.23	0.66
1:X:617:U:H5	1:X:632:A:C2	2.14	0.66
12:J:15:ARG:HD2	12:J:74:PRO:HD2	1.77	0.66
25:W:4:LYS:HG2	25:W:52:GLU:HB3	1.78	0.65
1:X:1673:C:C5'	4:B:136:ARG:HD3	2.26	0.65
2:Y:45:C:H2'	6:D:92:ARG:NH1	2.10	0.65
4:B:194:GLY:HA2	15:M:2:GLN:HB3	1.77	0.65
1:X:1810:U:H2'	3:A:157:ARG:HD3	1.78	0.65
1:X:2551:A:N7	4:B:145:LYS:HB2	2.10	0.65
1:X:2266:A:H62	1:X:2323:U:H3	1.43	0.65
1:X:320:A:N3	1:X:340:G:O2'	2.29	0.65
1:X:1811:A:H5''	3:A:161:THR:HG21	1.78	0.65
1:X:1673:C:H2'	1:X:1674:C:C6	2.31	0.64
1:X:797:A:C5	3:A:229:VAL:HG21	2.31	0.64
11:I:17:LYS:O	11:I:18:ARG:HB2	1.97	0.64
20:R:25:LEU:H	20:R:80:LYS:HA	1.62	0.64
24:V:25:LEU:HD21	24:V:47:ARG:HG2	1.78	0.64
12:J:48:ILE:HD12	12:J:71:PRO:HG3	1.80	0.64
5:C:48:ARG:C	5:C:50:GLN:H	2.00	0.64
1:X:1744:G:OP1	15:M:100:ARG:HD2	1.97	0.64
1:X:742:G:C6	3:A:208:LYS:HB3	2.33	0.64
12:J:28:VAL:HG23	12:J:137:VAL:HB	1.80	0.64
16:N:66:ASN:HB2	16:N:70:ARG:NH1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1609:G:H2'	1:X:1610:A:C8	2.32	0.64
1:X:482:A:H2'	1:X:483:A:O4'	1.96	0.64
12:J:28:VAL:HG12	12:J:29:ALA:H	1.63	0.63
1:X:1745:C:P	15:M:101:ARG:HH22	2.20	0.63
1:X:1582:A:OP1	3:A:211:ARG:NH2	2.31	0.63
1:X:841:G:H2'	1:X:842:A:C8	2.33	0.63
1:X:764:A:H5'	18:P:111:ARG:HA	1.79	0.63
1:X:2653:A:O2'	10:H:41:ASN:ND2	2.32	0.63
1:X:800:U:H5''	1:X:801:A:H5'	1.81	0.63
1:X:1674:C:H2'	1:X:1675:C:C6	2.34	0.63
15:M:60:SER:HB3	15:M:63:ARG:HH22	1.64	0.62
1:X:451:A:H2'	1:X:452:G:C8	2.34	0.62
3:A:67:PHE:HB3	3:A:153:ALA:H	1.64	0.62
18:P:32:ARG:HA	18:P:121:THR:HG22	1.81	0.62
4:B:152:LYS:H	9:G:106:TYR:HB3	1.64	0.62
5:C:176:ASN:HB3	5:C:179:ASP:HB2	1.81	0.62
11:I:108:LEU:HD23	11:I:129:ALA:HB1	1.82	0.62
4:B:152:LYS:HB2	9:G:106:TYR:CB	2.27	0.62
23:U:32:ARG:HG2	23:U:33:LYS:N	2.13	0.62
21:S:3:LEU:HD11	21:S:56:VAL:HG13	1.80	0.62
1:X:797:A:N7	3:A:229:VAL:HG21	2.15	0.62
6:D:143:TYR:HA	6:D:146:VAL:HG22	1.82	0.62
24:V:28:LEU:HD12	24:V:43:VAL:HG22	1.81	0.62
1:X:1753:A:O5'	1:X:1753:A:H8	1.82	0.61
11:I:28:LYS:NZ	11:I:36:GLY:HA2	2.16	0.61
13:K:3:HIS:HB3	13:K:5:LYS:HD2	1.81	0.61
10:H:124:MET:O	10:H:127:VAL:HG12	2.00	0.61
2:Y:28:A:H8	2:Y:29:C:C5	2.17	0.61
23:U:51:ILE:HA	23:U:59:THR:O	2.01	0.61
1:X:670:U:H2'	1:X:671:A:C8	2.35	0.61
1:X:2083:G:H1	1:X:2172:U:H3	1.48	0.61
1:X:746:G:N7	1:X:774:A:C6	2.69	0.61
25:W:7:ARG:HB2	25:W:50:LEU:HA	1.82	0.61
1:X:341:A:O2'	1:X:342:G:H8	1.83	0.61
1:X:564:U:H2'	1:X:565:A:C8	2.36	0.61
1:X:1574:A:O2'	1:X:1575:C:H3'	2.00	0.61
23:U:52:ARG:NE	23:U:79:GLU:HA	2.16	0.60
1:X:226:C:OP2	1:X:2373:C:O2'	2.19	0.60
1:X:450:C:H2'	1:X:451:A:C8	2.35	0.60
1:X:1745:C:OP1	15:M:101:ARG:NH2	2.33	0.60
15:M:17:GLU:O	15:M:21:THR:OG1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1437:A:H2'	1:X:1438:G:H8	1.64	0.60
3:A:223:GLY:HA2	3:A:226:MET:SD	2.40	0.60
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.83	0.60
1:X:512:A:H4'	18:P:15:LYS:HB3	1.83	0.60
5:C:47:THR:HA	5:C:82:VAL:HB	1.83	0.60
12:J:62:GLY:HA3	12:J:64:LYS:HE3	1.84	0.60
1:X:2543:A:H5'	1:X:2627:G:H4'	1.82	0.60
1:X:960:U:H2'	1:X:961:G:C8	2.37	0.60
5:C:176:ASN:HD22	5:C:179:ASP:H	1.48	0.60
1:X:504:G:H4'	18:P:27:VAL:HG12	1.84	0.60
1:X:412:U:H5''	23:U:68:ARG:HH22	1.67	0.60
1:X:168:A:H2'	1:X:169:C:H6	1.67	0.59
5:C:34:GLN:HB3	5:C:38:ARG:HH11	1.66	0.59
1:X:2484:G:H22	32:X:2929:1F4:H56	1.67	0.59
5:C:54:THR:HG21	5:C:72:ARG:HB3	1.84	0.59
1:X:954:U:OP2	11:I:38:LYS:HG2	2.01	0.59
1:X:2528:G:H2'	1:X:2529:G:H8	1.66	0.59
4:B:50:GLY:HA3	4:B:75:THR:HG21	1.85	0.59
1:X:38:G:H21	5:C:42:THR:HG21	1.66	0.59
1:X:1782:A:N6	1:X:1820:G:O2'	2.35	0.59
1:X:530:G:H2'	1:X:531:G:C8	2.37	0.59
16:N:66:ASN:HB2	16:N:70:ARG:HH11	1.67	0.59
18:P:27:VAL:HG23	18:P:125:THR:HG22	1.85	0.59
20:R:45:LYS:HA	20:R:76:LEU:O	2.02	0.59
18:P:40:LEU:HB3	26:Z:25:LEU:HD13	1.84	0.59
21:S:93:GLU:HB3	21:S:121:GLN:HG3	1.83	0.59
10:H:78:SER:HA	10:H:91:PHE:O	2.03	0.59
1:X:187:U:H2'	1:X:188:G:C8	2.37	0.59
17:O:36:LYS:HE2	17:O:56:VAL:HG22	1.85	0.58
22:T:45:PHE:HD2	22:T:77:ARG:HB3	1.67	0.58
1:X:1885:C:H4'	3:A:244:ARG:HD2	1.83	0.58
3:A:252:LYS:CD	3:A:253:PRO:HD3	2.32	0.58
16:N:66:ASN:CB	16:N:76:TYR:H	2.17	0.58
1:X:689:A:H2	1:X:815:A:H61	1.51	0.58
1:X:165:G:H2'	1:X:166:G:O4'	2.04	0.58
5:C:38:ARG:HH12	5:C:176:ASN:HD21	1.51	0.58
12:J:40:PRO:HB3	12:J:99:LYS:HD2	1.86	0.58
1:X:501:G:H2'	1:X:502:A:H8	1.65	0.58
1:X:2504:G:H21	30:4:1:MET:HE2	1.67	0.58
4:B:4:ILE:HG22	4:B:96:PHE:HE1	1.67	0.58
15:M:82:PRO:HG2	15:M:85:SER:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1030:U:HO2'	1:X:1032:A:H2	1.50	0.58
1:X:1999:U:O2'	26:Z:7:PRO:O	2.21	0.58
1:X:553:C:H42	1:X:559:C:H42	1.49	0.58
1:X:1656:U:H4'	1:X:2678:C:H4'	1.84	0.58
4:B:26:VAL:HG11	4:B:198:LEU:HD11	1.85	0.58
1:X:1584:G:N3	3:A:58:HIS:CE1	2.72	0.58
1:X:742:G:H2'	1:X:1766:U:H1'	1.85	0.58
1:X:405:C:H2'	1:X:406:G:H8	1.69	0.58
6:D:123:ASP:HB3	6:D:127:ASN:HB2	1.83	0.58
1:X:1505:U:HO2'	1:X:1506:C:H6	1.51	0.58
1:X:114:C:O2'	1:X:124:A:N3	2.37	0.57
1:X:1468:A:H5'	1:X:1472:C:N4	2.19	0.57
20:R:48:VAL:HG12	20:R:50:GLY:H	1.69	0.57
23:U:48:LYS:HG2	23:U:49:LYS:H	1.68	0.57
1:X:1071:U:H4'	1:X:1072:U:H3'	1.85	0.57
5:C:58:MET:HB2	5:C:70:GLY:O	2.04	0.57
5:C:119:ALA:H	5:C:189:ASP:HA	1.69	0.57
1:X:1040:A:H5''	12:J:129:GLN:HE22	1.69	0.57
1:X:482:A:O5'	1:X:482:A:H8	1.88	0.57
23:U:56:GLN:HE21	23:U:57:VAL:HG23	1.70	0.57
7:E:127:GLU:HG3	7:E:130:ARG:HB2	1.87	0.57
12:J:25:GLY:HA3	12:J:102:ARG:HA	1.87	0.57
23:U:48:LYS:CG	23:U:49:LYS:N	2.68	0.57
25:W:12:ARG:HG3	25:W:50:LEU:HD21	1.85	0.57
1:X:1437:A:H2'	1:X:1438:G:C8	2.40	0.57
1:X:712:A:H2'	1:X:713:G:O4'	2.05	0.57
5:C:43:ALA:CB	5:C:86:PRO:HB2	2.29	0.57
10:H:13:ASN:HD21	10:H:109:ARG:HG2	1.70	0.57
1:X:2081:U:H3	1:X:2174:G:H1	1.53	0.57
19:Q:68:PHE:O	19:Q:70:GLY:N	2.38	0.56
1:X:1845:A:H2'	1:X:1846:A:C8	2.40	0.56
1:X:1699:A:H61	1:X:1723:U:H3	1.51	0.56
1:X:1787:U:H2'	1:X:1788:C:C6	2.41	0.56
1:X:829:C:H2'	1:X:830:C:C6	2.40	0.56
3:A:36:ALA:HB1	3:A:62:TYR:O	2.04	0.56
1:X:1982:C:H5''	1:X:2703:C:O2'	2.05	0.56
1:X:1033:G:H22	1:X:1153:A:H2	1.53	0.56
14:L:27:LEU:HD23	14:L:44:ASP:HA	1.87	0.56
1:X:1173:G:H4'	17:O:22:VAL:HG23	1.86	0.56
23:U:14:VAL:O	23:U:15:VAL:HG22	2.06	0.56
1:X:559:C:H2'	1:X:560:G:C1'	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:149:LEU:HD11	5:C:170:LEU:HD13	1.87	0.56
1:X:530:G:H2'	1:X:531:G:H8	1.69	0.56
1:X:1268:U:C2	5:C:66:ASN:HA	2.41	0.56
13:K:3:HIS:CE1	13:K:5:LYS:HZ2	2.23	0.56
20:R:22:VAL:HG11	20:R:80:LYS:HD2	1.88	0.56
1:X:2653:A:H2'	10:H:41:ASN:ND2	2.21	0.56
1:X:215:G:H21	1:X:632:A:H8	1.52	0.56
1:X:1348:C:H2'	1:X:1349:A:C8	2.40	0.56
1:X:2266:A:N6	1:X:2323:U:H3	2.04	0.56
11:I:97:ARG:O	11:I:98:LEU:HB2	2.06	0.55
1:X:2516:U:H2'	1:X:2517:C:C6	2.40	0.55
32:X:2929:1F4:O18	32:X:2929:1F4:H9	2.06	0.55
16:N:66:ASN:HB3	16:N:76:TYR:CB	2.35	0.55
3:A:38:PRO:HA	3:A:61:LEU:HD23	1.88	0.55
1:X:1454:U:H2'	1:X:1455:C:C6	2.41	0.55
1:X:1468:A:H5'	1:X:1472:C:H41	1.71	0.55
1:X:187:U:H2'	1:X:188:G:H8	1.70	0.55
20:R:52:ASN:HD21	20:R:71:GLN:HE21	1.55	0.55
1:X:1348:C:H2'	1:X:1349:A:H8	1.71	0.55
1:X:1770:U:C5	1:X:1775:A:N7	2.62	0.55
1:X:1882:G:H21	1:X:1885:C:H41	1.53	0.55
1:X:1948:C:H5''	1:X:1949:A:H2'	1.89	0.55
1:X:1595:A:H2'	1:X:1596:A:O4'	2.07	0.55
1:X:2212:U:H2'	1:X:2213:G:C8	2.41	0.55
16:N:84:LYS:HG3	16:N:92:ARG:HH22	1.70	0.55
22:T:41:ARG:HA	22:T:41:ARG:HE	1.72	0.55
6:D:104:ILE:HA	6:D:108:LEU:HD12	1.88	0.55
5:C:136:TRP:O	5:C:140:ASN:ND2	2.40	0.54
9:G:106:TYR:O	9:G:110:LEU:HG	2.06	0.54
1:X:559:C:C2'	1:X:560:G:O4'	2.54	0.54
1:X:774:A:H8	1:X:774:A:O5'	1.90	0.54
18:P:97:VAL:HG22	18:P:124:ILE:HG23	1.87	0.54
16:N:37:GLN:HA	16:N:40:LEU:HD12	1.90	0.54
1:X:75:C:H5''	24:V:48:ARG:HG3	1.89	0.54
1:X:1032:A:H3'	1:X:1032:A:C8	2.42	0.54
1:X:2484:G:N2	32:X:2929:1F4:H56	2.22	0.54
1:X:1135:C:H2'	1:X:1136:G:O4'	2.06	0.54
1:X:333:A:H2'	5:C:162:ARG:HH12	1.72	0.54
1:X:1264:C:OP1	16:N:10:ARG:HG3	2.08	0.54
1:X:2659:C:H5'	4:B:189:PRO:HA	1.90	0.54
3:A:60:ARG:HD3	3:A:86:PRO:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:95:LEU:HD23	5:C:96:PRO:HD2	1.90	0.54
8:F:79:ARG:HG2	8:F:84:ILE:HB	1.90	0.54
1:X:219:G:N2	1:X:231:G:H2'	2.22	0.54
32:X:2929:1F4:C54	32:X:2929:1F4:H18	2.38	0.54
21:S:91:PRO:HG2	21:S:125:PRO:HD2	1.90	0.54
1:X:2196:U:H5'	1:X:2197:U:OP2	2.08	0.54
5:C:148:VAL:HG13	5:C:185:ARG:HB2	1.90	0.54
9:G:67:ARG:CG	9:G:70:PHE:HA	2.37	0.54
1:X:29:U:H5''	16:N:7:GLY:HA2	1.90	0.54
1:X:356:A:H2'	1:X:357:A:C8	2.43	0.54
1:X:2627:G:H2'	1:X:2628:C:O4'	2.08	0.54
6:D:80:ARG:HD3	6:D:83:MET:HB2	1.91	0.53
10:H:77:THR:HA	10:H:94:ASN:HB3	1.89	0.53
16:N:6:THR:O	16:N:9:VAL:HG23	2.08	0.53
21:S:123:VAL:HG23	21:S:161:ALA:HB2	1.90	0.53
32:X:2929:1F4:C39	32:X:2929:1F4:H9	2.38	0.53
1:X:760:U:O2	1:X:1997:A:H1'	2.08	0.53
1:X:171:G:H2'	1:X:172:A:O4'	2.08	0.53
1:X:2482:A:H4'	1:X:2483:U:OP1	2.08	0.53
3:A:182:LEU:HD12	3:A:269:PHE:HB2	1.90	0.53
13:K:87:TYR:CE1	13:K:94:TYR:HD2	2.27	0.53
15:M:29:PRO:HB2	15:M:99:VAL:HG21	1.90	0.53
21:S:95:SER:HB3	21:S:119:ASN:HD22	1.74	0.53
1:X:1134:C:H2'	1:X:1135:C:H6	1.74	0.53
1:X:2459:C:H2'	1:X:2459:C:O2	2.08	0.53
1:X:1673:C:H5'	4:B:136:ARG:HD3	1.91	0.53
9:G:132:PHE:HB2	9:G:145:HIS:CE1	2.44	0.53
1:X:1223:G:H5'	1:X:1225:G:O4'	2.08	0.53
4:B:5:LEU:HG	4:B:195:LEU:HD11	1.91	0.53
5:C:48:ARG:C	5:C:50:GLN:N	2.61	0.53
10:H:83:ARG:CZ	10:H:89:ILE:HD11	2.38	0.53
14:L:38:ILE:HG13	14:L:39:TYR:N	2.17	0.53
20:R:26:SER:H	20:R:30:LYS:HG3	1.73	0.53
21:S:6:LYS:N	21:S:7:PRO:HD3	2.20	0.53
1:X:1076:U:H3	1:X:1080:A:H2'	1.74	0.53
1:X:732:G:H2'	1:X:733:G:C8	2.43	0.53
2:Y:9:G:H1	2:Y:116:C:H42	1.56	0.53
11:I:102:LYS:O	11:I:104:ARG:N	2.35	0.53
18:P:62:ARG:HE	26:Z:25:LEU:HD11	1.74	0.53
1:X:555:U:H5'	1:X:556:A:C8	2.43	0.53
1:X:761:G:OP2	18:P:109:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:32:ARG:HG2	23:U:33:LYS:H	1.72	0.53
1:X:2041:A:H61	32:X:2929:1F4:H46	1.73	0.53
1:X:633:G:H2'	1:X:634:G:H8	1.73	0.53
3:A:45:ASN:CG	3:A:46:ARG:H	2.12	0.52
9:G:105:GLY:O	9:G:106:TYR:C	2.46	0.52
25:W:3:ILE:HG23	25:W:51:LEU:HD22	1.92	0.52
1:X:1287:A:H2'	1:X:1288:A:H5''	1.91	0.52
1:X:1468:A:O5'	1:X:1468:A:C8	2.62	0.52
1:X:2225:G:H2'	1:X:2226:A:C8	2.43	0.52
1:X:2270:U:H2'	1:X:2271:C:C6	2.43	0.52
1:X:577:U:H5''	1:X:956:A:N6	2.23	0.52
10:H:70:VAL:CG2	10:H:98:ILE:HG23	2.38	0.52
1:X:796:A:H8	1:X:797:A:H4'	1.74	0.52
3:A:79:VAL:HG21	3:A:111:LEU:HD22	1.91	0.52
4:B:131:SER:O	4:B:132:LYS:HG2	2.10	0.52
1:X:1378:A:H1'	23:U:16:ASN:HD21	1.74	0.52
1:X:1998:A:O5'	1:X:1998:A:H8	1.92	0.52
3:A:245:VAL:HG12	3:A:250:TRP:O	2.09	0.52
1:X:1039:A:N6	1:X:1136:G:H2'	2.24	0.52
1:X:2505:G:H1	1:X:2516:U:H3	1.58	0.52
4:B:31:CYS:HB3	4:B:49:ILE:HG23	1.90	0.52
12:J:37:ALA:O	12:J:100:PRO:HA	2.09	0.52
1:X:110:U:H3'	1:X:111:G:C8	2.44	0.52
1:X:1609:G:H2'	1:X:1610:A:H8	1.73	0.52
1:X:768:U:H2'	1:X:769:C:O4'	2.09	0.52
1:X:760:U:C5	26:Z:3:LYS:HG3	2.44	0.52
1:X:2860:C:H2'	1:X:2861:A:O4'	2.09	0.52
8:F:117:ALA:HB1	8:F:122:ALA:HB1	1.92	0.52
13:K:17:ARG:HH11	13:K:20:LEU:CD2	2.23	0.52
14:L:8:ARG:HG3	14:L:9:ARG:H	1.74	0.52
23:U:51:ILE:HG23	23:U:59:THR:HA	1.92	0.52
23:U:51:ILE:HG12	23:U:59:THR:HB	1.92	0.52
1:X:1859:A:H2'	1:X:1860:A:C8	2.45	0.52
1:X:2372:A:H5''	11:I:61:PRO:HB3	1.92	0.52
1:X:568:G:H2'	1:X:569:C:O4'	2.09	0.52
1:X:83:A:H2	1:X:97:U:O2	1.92	0.52
2:Y:46:G:H5'	6:D:92:ARG:HH12	1.73	0.52
4:B:152:LYS:H	9:G:106:TYR:CB	2.22	0.52
10:H:27:SER:HA	10:H:50:ILE:HD12	1.90	0.52
13:K:28:LEU:HD12	13:K:48:VAL:HG21	1.92	0.52
17:O:40:VAL:HG12	17:O:43:GLU:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1465:G:N2	1:X:1477:C:O2	2.41	0.52
1:X:1856:U:OP1	1:X:2389:G:O2'	2.26	0.52
1:X:465:C:O2'	1:X:483:A:N6	2.42	0.52
14:L:36:LYS:HB3	14:L:64:LYS:HB2	1.92	0.52
1:X:504:G:H21	18:P:78:ASN:HD21	1.57	0.52
1:X:1673:C:H5''	4:B:136:ARG:HD3	1.91	0.52
1:X:2528:G:H5''	1:X:2528:G:C8	2.45	0.52
1:X:2594:U:C2	26:Z:7:PRO:HA	2.45	0.52
4:B:16:LYS:HB2	4:B:21:ILE:HD11	1.92	0.52
1:X:1623:C:H4'	1:X:1624:A:O5'	2.10	0.52
1:X:216:U:H2'	1:X:217:U:O4'	2.10	0.52
1:X:450:C:H2'	1:X:451:A:H8	1.73	0.52
4:B:116:VAL:CG2	4:B:136:ARG:HE	2.15	0.51
3:A:43:ARG:HB3	3:A:54:ILE:HG12	1.91	0.51
1:X:400:U:H5	23:U:21:ARG:HH12	1.57	0.51
1:X:1804:U:H2'	1:X:1805:G:H8	1.73	0.51
1:X:2797:G:OP2	13:K:3:HIS:NE2	2.42	0.51
2:Y:43:G:H5'	2:Y:44:C:H5''	1.91	0.51
1:X:413:G:H8	1:X:413:G:O5'	1.93	0.51
1:X:611:C:H5''	1:X:611:C:H6	1.75	0.51
1:X:627:A:H2'	1:X:628:A:C8	2.46	0.51
1:X:1586:A:H5'	3:A:38:PRO:HG3	1.93	0.51
9:G:93:LYS:HB3	9:G:96:ASP:HB3	1.92	0.51
15:M:69:ARG:HG3	15:M:78:GLU:HG3	1.93	0.51
20:R:59:LYS:HG2	20:R:62:MET:HB3	1.93	0.51
21:S:117:VAL:HG22	21:S:168:VAL:HA	1.91	0.51
5:C:24:SER:HA	5:C:27:LEU:HD12	1.93	0.51
1:X:1016:C:O2'	9:G:56:THR:HG21	2.11	0.51
32:X:2929:1F4:C23	32:X:2929:1F4:C41	2.88	0.51
1:X:388:G:H2'	1:X:389:G:H8	1.75	0.51
1:X:451:A:H2'	1:X:452:G:H8	1.74	0.51
6:D:114:PHE:HZ	6:D:176:PRO:HG2	1.74	0.51
6:D:4:LEU:HG	6:D:5:LYS:H	1.74	0.51
1:X:2545:A:H61	10:H:40:GLY:HA3	1.74	0.51
1:X:2042:A:OP1	5:C:66:ASN:ND2	2.44	0.51
7:E:6:LYS:HB3	7:E:69:ARG:HD3	1.93	0.51
1:X:699:G:C8	1:X:699:G:H5'	2.46	0.51
4:B:146:THR:OG1	4:B:147:PRO:HD3	2.11	0.51
17:O:8:GLY:H	17:O:20:ILE:HD13	1.75	0.51
1:X:2289:A:H3'	1:X:2290:A:H8	1.75	0.51
1:X:840:U:O2	1:X:2225:G:H4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:44:ARG:HE	15:M:46:ARG:HH21	1.58	0.51
1:X:1542:G:N2	1:X:1562:G:H1	1.94	0.51
1:X:334:G:OP1	1:X:349:G:N2	2.44	0.51
3:A:58:HIS:O	3:A:58:HIS:ND1	2.44	0.50
20:R:105:ARG:HH22	20:R:112:LYS:HA	1.76	0.50
1:X:1736:C:H2'	1:X:1737:G:C8	2.46	0.50
1:X:1584:G:H4'	3:A:59:LYS:HG2	1.94	0.50
5:C:22:VAL:HG22	5:C:106:MET:HG3	1.92	0.50
1:X:935:C:H2'	1:X:936:A:C8	2.45	0.50
17:O:15:SER:HA	17:O:95:ILE:O	2.11	0.50
21:S:3:LEU:HD13	21:S:32:PHE:HB3	1.93	0.50
1:X:1454:U:H2'	1:X:1455:C:H6	1.76	0.50
4:B:4:ILE:HG12	4:B:28:ALA:HB1	1.94	0.50
4:B:61:LYS:HB3	4:B:62:PRO:HD3	1.93	0.50
12:J:26:ASP:HB3	12:J:68:ARG:HH22	1.76	0.50
1:X:2271:C:P	14:L:18:ARG:HH21	2.35	0.50
23:U:52:ARG:HD3	23:U:70:LEU:HD22	1.92	0.50
1:X:1834:G:H1	1:X:1881:U:H3	1.59	0.50
32:X:2929:1F4:C50	32:X:2929:1F4:C52	2.90	0.50
4:B:35:GLN:HB2	4:B:48:GLN:HB3	1.93	0.50
1:X:1142:G:C1'	9:G:103:TYR:HD2	2.25	0.50
13:K:17:ARG:HH11	13:K:20:LEU:HD22	1.76	0.50
16:N:24:PHE:O	16:N:29:SER:HB3	2.11	0.50
1:X:1656:U:H2'	1:X:1657:A:H5''	1.94	0.50
1:X:2002:A:N7	26:Z:9:LYS:HD2	2.26	0.50
1:X:620:G:N2	1:X:630:G:H1'	2.26	0.50
3:A:246:PRO:HD2	3:A:249:PRO:O	2.12	0.50
3:A:182:LEU:HB2	3:A:268:ARG:O	2.11	0.50
5:C:148:VAL:HB	5:C:167:VAL:HG12	1.93	0.50
9:G:132:PHE:CE2	9:G:145:HIS:HB2	2.47	0.50
1:X:1685:A:H5''	10:H:5:GLN:HG2	1.93	0.50
1:X:969:U:H5''	12:J:17:ARG:HH11	1.77	0.50
15:M:33:VAL:HG22	15:M:51:GLU:HB2	1.93	0.50
20:R:92:THR:HB	20:R:95:ARG:HH22	1.75	0.50
21:S:51:LEU:HB3	21:S:65:LEU:HD12	1.94	0.50
1:X:884:C:H2'	1:X:885:A:H8	1.77	0.50
5:C:164:VAL:C	5:C:166:TRP:H	2.15	0.49
1:X:2056:C:H4'	3:A:228:PRO:HB2	1.93	0.49
26:Z:30:LEU:HD22	26:Z:39:LYS:HB3	1.94	0.49
23:U:48:LYS:HG2	23:U:49:LYS:N	2.27	0.49
1:X:2861:A:O2'	26:Z:31:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:127:PRO:C	21:S:129:ARG:H	2.16	0.49
1:X:504:G:H4'	18:P:27:VAL:CG1	2.42	0.49
5:C:4:ILE:HG22	5:C:13:ARG:HH21	1.77	0.49
8:F:112:MET:HA	8:F:115:LEU:HD12	1.94	0.49
14:L:15:ARG:HD2	14:L:91:ARG:HD2	1.95	0.49
1:X:1448:A:H61	1:X:1574:A:N6	1.93	0.49
1:X:1326:U:H2'	1:X:1626:A:C2	2.48	0.49
1:X:1632:A:H5'	1:X:1632:A:H8	1.77	0.49
1:X:1979:C:H4'	1:X:1980:A:OP1	2.13	0.49
1:X:2597:G:H21	4:B:150:VAL:HG11	1.77	0.49
26:Z:45:ILE:HG21	26:Z:57:VAL:HG23	1.94	0.49
3:A:66:ASP:HB3	3:A:105:ILE:HD12	1.93	0.49
10:H:113:PRO:HB3	10:H:134:LEU:HD12	1.94	0.49
1:X:2653:A:C2'	10:H:41:ASN:ND2	2.75	0.49
13:K:11:ASN:HD21	13:K:17:ARG:NH1	2.09	0.49
1:X:1089:C:H5'	8:F:132:ARG:HH12	1.77	0.49
1:X:2546:G:H2'	1:X:2547:C:C6	2.48	0.49
9:G:90:LEU:HD23	9:G:94:LYS:HA	1.94	0.49
21:S:56:VAL:HG12	21:S:57:GLU:H	1.78	0.49
21:S:5:ALA:HB1	21:S:7:PRO:HD3	1.94	0.49
1:X:2039:G:H2'	1:X:2039:G:N3	2.28	0.49
1:X:1750:A:H1'	1:X:2690:A:C2	2.47	0.49
1:X:347:C:H4'	20:R:15:HIS:CD2	2.48	0.49
2:Y:50:U:OP1	14:L:94:TYR:HA	2.13	0.49
3:A:58:HIS:O	3:A:59:LYS:HB3	2.11	0.49
16:N:74:MET:HG2	16:N:78:THR:HG22	1.94	0.49
2:Y:92:G:H8	2:Y:92:G:OP2	1.95	0.49
3:A:164:GLN:HB3	3:A:176:ARG:HB3	1.94	0.49
10:H:112:GLY:O	10:H:131:PRO:HD2	2.13	0.49
16:N:66:ASN:HD22	16:N:70:ARG:HH12	1.60	0.49
1:X:1030:U:H3	1:X:1153:A:H62	1.61	0.49
1:X:1478:U:H2'	1:X:1479:G:H8	1.78	0.49
1:X:2035:G:H4'	4:B:143:GLN:O	2.13	0.49
1:X:229:G:OP1	11:I:49:PHE:HE1	1.96	0.49
13:K:87:TYR:HE1	13:K:94:TYR:HD2	1.59	0.49
16:N:75:ASN:ND2	16:N:78:THR:H	2.10	0.49
1:X:1509:A:H8	1:X:1510:A:C8	2.30	0.49
4:B:27:LEU:HD23	4:B:51:TYR:OH	2.12	0.48
17:O:71:ILE:HD11	17:O:86:HIS:HB2	1.94	0.48
1:X:1469:U:P	1:X:1471:G:OP2	2.71	0.48
1:X:2779:C:H2'	1:X:2780:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:60:ILE:HD12	6:D:61:THR:HG23	1.95	0.48
1:X:643:A:H4'	11:I:67:ASN:HB3	1.95	0.48
1:X:1333:G:N2	1:X:1344:C:N4	2.61	0.48
32:X:2929:1F4:H3	32:X:2929:1F4:O18	2.12	0.48
1:X:463:C:H42	1:X:467:U:H5	1.60	0.48
1:X:793:G:H21	1:X:796:A:H62	1.61	0.48
3:A:37:LEU:HD13	3:A:38:PRO:HD2	1.95	0.48
1:X:611:C:H4'	5:C:98:GLN:HE22	1.79	0.48
18:P:102:THR:HG21	18:P:118:LYS:HB3	1.95	0.48
1:X:1608:U:H2'	1:X:1609:G:C8	2.48	0.48
1:X:2857:C:H5'	13:K:96:ARG:HG3	1.94	0.48
3:A:165:VAL:HA	3:A:175:VAL:HG12	1.94	0.48
11:I:30:ALA:HB3	11:I:34:HIS:HE1	1.70	0.48
16:N:50:ARG:O	16:N:53:LYS:HG2	2.13	0.48
25:W:4:LYS:CG	25:W:52:GLU:HB3	2.43	0.48
1:X:1478:U:H2'	1:X:1479:G:C8	2.48	0.48
1:X:1515:U:H2'	1:X:1516:A:H8	1.79	0.48
1:X:794:A:H5'	3:A:218:LYS:NZ	2.29	0.48
11:I:32:ARG:HD2	17:O:79:GLN:NE2	2.29	0.48
23:U:48:LYS:HG3	23:U:49:LYS:H	1.79	0.48
1:X:1202:U:H2'	1:X:1203:A:H8	1.78	0.48
1:X:2821:G:H2'	1:X:2822:U:C6	2.49	0.48
1:X:654:A:H2	1:X:655:A:H3'	1.78	0.48
1:X:958:G:H2'	1:X:959:C:C6	2.49	0.48
1:X:1093:U:H5'	8:F:117:ALA:HA	1.96	0.48
17:O:10:LYS:HG3	17:O:11:GLN:HG2	1.96	0.48
20:R:38:LEU:HB3	20:R:47:VAL:HB	1.95	0.48
1:X:82:G:N1	1:X:100:G:H2'	2.29	0.48
1:X:503:G:H2'	1:X:504:G:O4'	2.14	0.48
3:A:118:ASN:HD22	3:A:119:ALA:N	2.12	0.48
14:L:31:VAL:HG21	14:L:100:VAL:HG23	1.96	0.48
1:X:1167:A:H61	16:N:48:ARG:HG2	1.79	0.48
20:R:23:ILE:HG22	20:R:33:THR:HB	1.95	0.48
1:X:527:C:OP1	26:Z:16:ARG:NH2	2.46	0.48
10:H:26:ASN:CB	10:H:38:GLY:H	2.26	0.48
11:I:130:ILE:HG22	11:I:140:VAL:HG21	1.96	0.48
1:X:1918:G:H1'	1:X:1947:G:N2	2.28	0.48
1:X:2045:A:O5'	1:X:2045:A:H8	1.96	0.48
1:X:621:U:H2'	1:X:622:U:C6	2.49	0.48
23:U:65:ASN:HA	23:U:68:ARG:HD3	1.96	0.48
6:D:8:TYR:O	6:D:12:VAL:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1497:C:C6	1:X:1497:C:H5''	2.50	0.47
1:X:1736:C:H2'	1:X:1737:G:H8	1.79	0.47
1:X:1687:C:OP2	1:X:2529:G:OP1	2.32	0.47
1:X:881:U:H2'	1:X:882:C:C6	2.49	0.47
23:U:52:ARG:HE	23:U:79:GLU:HA	1.77	0.47
24:V:42:ARG:NH1	24:V:45:GLN:OE1	2.47	0.47
1:X:1515:U:H2'	1:X:1516:A:C8	2.49	0.47
2:Y:21:C:H2'	2:Y:22:U:O4'	2.13	0.47
10:H:116:ARG:HH11	15:M:38:LYS:HD3	1.79	0.47
18:P:57:LEU:HD13	18:P:69:ALA:HA	1.96	0.47
1:X:1406:A:N6	19:Q:15:LYS:HG2	2.29	0.47
1:X:1674:C:H2'	1:X:1675:C:H6	1.76	0.47
32:X:2929:1F4:H11	32:X:2929:1F4:C41	2.44	0.47
3:A:118:ASN:HD22	3:A:119:ALA:H	1.61	0.47
7:E:67:LEU:O	7:E:71:LEU:HG	2.15	0.47
9:G:67:ARG:HE	9:G:70:PHE:HA	1.78	0.47
11:I:62:LYS:NZ	11:I:64:GLY:HA3	2.28	0.47
20:R:22:VAL:HG13	20:R:81:VAL:O	2.14	0.47
25:W:1:MET:HB3	25:W:34:VAL:HG12	1.96	0.47
4:B:133:LYS:HG2	4:B:137:ARG:HB3	1.96	0.47
1:X:1673:C:H5'	4:B:136:ARG:HH11	1.78	0.47
1:X:2362:G:H2'	1:X:2363:G:C8	2.49	0.47
3:A:186:HIS:HB2	3:A:188:GLU:CG	2.44	0.47
11:I:32:ARG:HD2	17:O:79:GLN:HE22	1.80	0.47
10:H:90:ARG:HG2	15:M:78:GLU:HB2	1.96	0.47
1:X:1168:G:O2'	25:W:28:ILE:HG12	2.15	0.47
1:X:1507:A:H2'	1:X:1508:G:H8	1.79	0.47
1:X:2394:G:H4'	11:I:65:PHE:HB3	1.96	0.47
1:X:588:G:H2'	1:X:589:C:H6	1.78	0.47
3:A:208:LYS:C	3:A:209:ALA:O	2.53	0.47
4:B:149:ARG:NH1	9:G:106:TYR:HB2	2.29	0.47
4:B:149:ARG:CZ	9:G:106:TYR:HD1	2.28	0.47
1:X:2014:A:C6	1:X:2477:C:H1'	2.49	0.47
1:X:388:G:H2'	1:X:389:G:C8	2.50	0.47
3:A:208:LYS:O	3:A:209:ALA:O	2.32	0.47
9:G:61:ARG:HH11	9:G:66:HIS:H	1.61	0.47
11:I:58:ALA:O	11:I:59:ARG:CB	2.62	0.47
21:S:131:PRO:HG3	21:S:155:PRO:HG2	1.97	0.47
21:S:23:ALA:HA	21:S:83:PHE:O	2.14	0.47
4:B:5:LEU:HD12	4:B:197:VAL:HG22	1.97	0.47
13:K:97:ILE:HA	13:K:112:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:38:LEU:HD23	17:O:47:PHE:HB3	1.96	0.47
1:X:203:G:H21	1:X:205:A:H62	1.63	0.47
1:X:2048:C:H1'	1:X:2428:U:O2	2.14	0.47
1:X:2493:U:H2'	1:X:2494:C:C6	2.50	0.47
1:X:588:G:H2'	1:X:589:C:C6	2.49	0.47
1:X:7:G:H2'	1:X:8:A:C8	2.50	0.47
6:D:40:LEU:HD21	6:D:87:ILE:HD12	1.96	0.47
19:Q:61:LYS:H	19:Q:72:ARG:HA	1.79	0.47
1:X:1255:A:H2'	1:X:1256:C:C6	2.50	0.47
1:X:1584:G:N3	3:A:58:HIS:HE1	2.10	0.47
6:D:63:GLN:HG3	6:D:95:ARG:HH21	1.79	0.47
16:N:49:ASP:HA	16:N:52:ASN:HB2	1.97	0.47
1:X:745:C:H2'	1:X:746:G:O4'	2.14	0.47
19:Q:12:ILE:H	19:Q:12:ILE:HD13	1.80	0.46
1:X:2653:A:H4'	10:H:42:LYS:HB2	1.97	0.46
1:X:609:U:H4'	11:I:18:ARG:HE	1.80	0.46
9:G:61:ARG:HG2	9:G:65:LYS:HE3	1.96	0.46
12:J:28:VAL:HG13	12:J:135:ARG:HG2	1.98	0.46
16:N:88:ILE:CG1	17:O:49:GLU:HB2	2.45	0.46
2:Y:94:G:H5'	21:S:74:ARG:HH12	1.79	0.46
9:G:116:ARG:HA	9:G:119:LEU:HD12	1.98	0.46
1:X:2604:G:H2'	1:X:2605:C:O4'	2.15	0.46
3:A:244:ARG:N	3:A:244:ARG:HD3	2.30	0.46
22:T:45:PHE:CD2	22:T:77:ARG:HB3	2.47	0.46
1:X:1329:U:H5'	1:X:1405:A:H1'	1.97	0.46
1:X:2286:G:C2	1:X:2287:G:H1'	2.50	0.46
9:G:66:HIS:HA	16:N:67:ALA:HB1	1.98	0.46
15:M:13:LEU:HD12	15:M:13:LEU:HA	1.70	0.46
20:R:35:LYS:HE3	20:R:37:LEU:HB3	1.98	0.46
21:S:19:ILE:HD12	21:S:79:ILE:HA	1.97	0.46
22:T:48:GLY:HA3	22:T:79:ILE:O	2.15	0.46
25:W:47:VAL:HB	25:W:50:LEU:HD12	1.98	0.46
1:X:1148:G:H2'	1:X:1149:G:O4'	2.14	0.46
1:X:118:U:H4'	1:X:119:G:H5''	1.97	0.46
1:X:876:A:H2'	1:X:877:G:C8	2.50	0.46
4:B:117:MET:HG3	4:B:136:ARG:HG3	1.98	0.46
11:I:32:ARG:HB3	17:O:79:GLN:NE2	2.31	0.46
12:J:109:GLY:HA3	21:S:112:LEU:HD21	1.97	0.46
16:N:72:HIS:HB2	16:N:110:VAL:HG11	1.96	0.46
1:X:2574:G:N2	1:X:2577:A:C8	2.82	0.46
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:63:ASN:HB3	14:L:66:ASP:HB2	1.96	0.46
19:Q:20:MET:HG2	19:Q:92:ALA:O	2.16	0.46
1:X:1169:C:H4'	25:W:28:ILE:O	2.16	0.46
1:X:1333:G:N2	1:X:1344:C:H41	2.14	0.46
1:X:1978:U:H1'	10:H:3:MET:HE1	1.97	0.46
1:X:2522:G:H2'	1:X:2523:G:C8	2.50	0.46
1:X:547:U:H2'	1:X:548:G:C8	2.50	0.46
1:X:649:G:H22	1:X:661:C:H1'	1.80	0.46
11:I:121:HIS:HA	11:I:141:VAL:HB	1.98	0.46
11:I:77:LEU:HD13	11:I:110:ALA:HA	1.98	0.46
1:X:1505:U:O2'	1:X:1506:C:H6	1.98	0.46
1:X:2691:C:O2'	1:X:2693:U:H5'	2.16	0.46
1:X:2784:A:C6	1:X:2866:A:C8	3.04	0.46
26:Z:33:CYS:HB2	26:Z:46:CYS:SG	2.56	0.46
1:X:333:A:H2'	5:C:162:ARG:NH1	2.30	0.46
1:X:609:U:H5'	11:I:18:ARG:HD3	1.97	0.46
1:X:540:G:H1'	1:X:2004:U:O2'	2.16	0.46
19:Q:66:GLY:O	19:Q:68:PHE:N	2.34	0.46
22:T:71:ASN:HD21	22:T:74:LYS:HG2	1.81	0.46
1:X:636:G:C8	1:X:636:G:H5''	2.51	0.46
17:O:25:LEU:HB2	17:O:32:LYS:HE2	1.98	0.45
1:X:1032:A:H3'	1:X:1032:A:H8	1.78	0.45
1:X:2062:U:H2'	1:X:2063:A:C8	2.52	0.45
1:X:2352:A:H2'	1:X:2353:G:H8	1.81	0.45
1:X:784:U:H2'	1:X:785:U:C6	2.51	0.45
4:B:32:PRO:HA	4:B:89:ASP:HB3	1.98	0.45
20:R:90:LYS:HB2	20:R:108:VAL:HG21	1.98	0.45
1:X:172:A:H61	1:X:175:C:H3'	1.81	0.45
1:X:240:U:H2'	1:X:241:C:O4'	2.16	0.45
6:D:106:ILE:HG21	6:D:139:PRO:HB3	1.98	0.45
12:J:42:TRP:CD1	12:J:97:VAL:HG12	2.51	0.45
12:J:21:ASP:HA	12:J:99:LYS:HE2	1.97	0.45
14:L:66:ASP:C	14:L:68:ALA:H	2.19	0.45
5:C:5:ASN:HB3	5:C:10:ASN:HA	1.99	0.45
1:X:523:A:O2'	16:N:11:ARG:HD2	2.16	0.45
25:W:19:THR:HG21	25:W:46:THR:HG22	1.98	0.45
1:X:1805:G:N3	3:A:50:THR:CG2	2.80	0.45
1:X:2210:C:OP1	23:U:45:ASN:HA	2.17	0.45
1:X:2371:A:H1'	11:I:59:ARG:HG3	1.97	0.45
1:X:2843:A:H5''	1:X:2843:A:C8	2.51	0.45
1:X:313:U:H2'	1:X:314:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:673:G:H5'	5:C:93:TYR:CD1	2.52	0.45
1:X:1673:C:H5'	4:B:136:ARG:NH1	2.31	0.45
1:X:1845:A:N1	1:X:2070:G:H1'	2.31	0.45
1:X:322:A:N6	1:X:339:U:H2'	2.31	0.45
1:X:428:A:H2'	1:X:429:C:O4'	2.17	0.45
1:X:631:G:H1	5:C:97:ARG:NH1	2.14	0.45
1:X:674:U:H2'	1:X:675:C:O4'	2.17	0.45
17:O:48:GLY:C	17:O:50:ASP:H	2.20	0.45
1:X:1234:C:H2'	1:X:1235:C:H6	1.82	0.45
1:X:1805:G:N3	3:A:50:THR:HG22	2.31	0.45
1:X:635:C:O2'	1:X:670:U:H5''	2.17	0.45
1:X:710:C:H2'	1:X:711:C:C6	2.52	0.45
2:Y:28:A:C8	2:Y:29:C:C5	3.02	0.45
3:A:83:GLU:N	3:A:92:ILE:O	2.46	0.45
2:Y:46:G:H4'	6:D:92:ARG:HH12	1.82	0.45
7:E:11:VAL:HG11	7:E:50:LEU:HD13	1.98	0.45
12:J:31:GLY:HA2	12:J:108:ALA:HB2	1.99	0.45
18:P:105:ARG:HB3	18:P:105:ARG:HE	1.64	0.45
20:R:105:ARG:NH2	20:R:112:LYS:HA	2.32	0.45
23:U:19:ILE:HA	23:U:42:GLN:HA	1.98	0.45
1:X:1832:G:H1	1:X:1885:C:N4	2.09	0.45
1:X:1981:A:H2'	1:X:1982:C:O4'	2.16	0.45
1:X:1997:A:H2'	1:X:1998:A:C8	2.51	0.45
3:A:134:ARG:HG3	3:A:135:PHE:HD2	1.81	0.45
5:C:74:VAL:HG23	5:C:76:THR:H	1.81	0.45
9:G:154:GLU:C	9:G:157:PRO:HD2	2.36	0.45
10:H:11:ALA:O	10:H:110:VAL:HA	2.17	0.45
12:J:42:TRP:CG	12:J:95:VAL:HG11	2.52	0.45
1:X:1573:G:H3'	1:X:1574:A:O4'	2.17	0.45
9:G:34:PRO:HA	9:G:69:ASP:CG	2.37	0.45
1:X:1164:C:H5'	16:N:76:TYR:CE2	2.52	0.45
1:X:2222:U:H2'	1:X:2223:U:C6	2.52	0.45
1:X:2579:A:H2'	1:X:2580:C:C6	2.52	0.45
1:X:2661:G:O6	1:X:2708:U:H1'	2.17	0.45
15:M:79:ARG:CG	15:M:79:ARG:NH1	2.68	0.45
23:U:22:GLY:HA3	23:U:39:LYS:HD2	1.98	0.45
1:X:593:C:N4	1:X:594:G:C6	2.85	0.45
1:X:640:C:C4'	1:X:660:G:H21	2.23	0.45
4:B:119:ARG:HG2	4:B:120:TRP:CE2	2.52	0.44
9:G:70:PHE:HB2	16:N:64:ARG:HE	1.83	0.44
20:R:97:GLN:HB2	20:R:101:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1045:G:N2	1:X:1133:G:H1'	2.31	0.44
1:X:1367:A:H2'	1:X:1368:G:O4'	2.17	0.44
1:X:636:G:O2'	1:X:669:G:H4'	2.17	0.44
3:A:79:VAL:HG21	3:A:111:LEU:CD2	2.47	0.44
1:X:1494:G:H2'	1:X:1495:G:O4'	2.17	0.44
1:X:1769:U:H2'	1:X:1775:A:N6	2.31	0.44
1:X:2252:A:H2'	1:X:2253:A:C8	2.52	0.44
3:A:147:LEU:HD22	3:A:183:ARG:HH22	1.82	0.44
3:A:208:LYS:HE3	3:A:208:LYS:HA	2.00	0.44
12:J:73:LYS:H	12:J:94:TRP:HD1	1.65	0.44
20:R:25:LEU:N	20:R:80:LYS:HA	2.30	0.44
1:X:1117:G:H2'	1:X:1118:G:H8	1.80	0.44
1:X:1202:U:H5'	17:O:78:VAL:HG22	1.98	0.44
1:X:1373:G:N2	1:X:2192:U:H3	2.15	0.44
1:X:2195:C:H5''	1:X:2195:C:H6	1.82	0.44
2:Y:72:C:H2'	2:Y:73:C:H6	1.82	0.44
1:X:1834:G:H1'	3:A:244:ARG:HH22	1.82	0.44
10:H:70:VAL:HG21	10:H:98:ILE:HG23	1.98	0.44
9:G:70:PHE:HB2	16:N:64:ARG:HG2	1.98	0.44
18:P:41:VAL:HG22	18:P:60:ILE:HG21	1.99	0.44
1:X:956:A:C4	1:X:2427:A:C2	3.06	0.44
1:X:796:A:H4'	1:X:2567:G:H4'	1.99	0.44
1:X:339:U:O4	1:X:343:A:C8	2.70	0.44
1:X:224:G:H4'	1:X:399:G:C5	2.52	0.44
3:A:231:HIS:ND1	3:A:247:VAL:HA	2.31	0.44
3:A:42:GLY:H	3:A:43:ARG:NH1	2.15	0.44
5:C:46:ARG:HD2	5:C:51:VAL:HB	1.99	0.44
12:J:98:VAL:HG11	12:J:104:MET:HG2	2.00	0.44
1:X:1833:U:H2'	1:X:1834:G:C8	2.53	0.44
1:X:358:C:H6	1:X:358:C:O5'	2.01	0.44
2:Y:89:G:N2	2:Y:92:G:C8	2.86	0.44
1:X:1819:U:OP2	3:A:222:ARG:NH2	2.50	0.44
1:X:2056:C:H5'	3:A:229:VAL:HG22	2.00	0.44
4:B:5:LEU:HD22	4:B:49:ILE:HG22	1.99	0.44
4:B:54:LYS:HD3	4:B:59:VAL:HG22	1.99	0.44
12:J:77:LYS:O	12:J:88:LYS:HD2	2.18	0.44
22:T:40:GLN:HE21	22:T:57:HIS:HB3	1.83	0.44
1:X:1524:C:H3'	1:X:1525:A:H8	1.82	0.44
1:X:2609:G:H2'	1:X:2610:G:C8	2.52	0.44
1:X:819:C:OP2	11:I:41:SER:HA	2.17	0.44
3:A:67:PHE:HB3	3:A:153:ALA:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:164:PHE:O	7:E:166:GLY:N	2.51	0.44
12:J:44:LYS:HB3	12:J:46:ASN:ND2	2.33	0.44
13:K:76:VAL:HA	13:K:79:VAL:HG12	2.00	0.44
1:X:1223:G:H5''	1:X:1224:A:H3'	2.00	0.44
1:X:1725:C:H42	1:X:1741:G:H1	1.64	0.44
1:X:2002:A:N1	1:X:2018:G:O6	2.51	0.44
1:X:490:A:N3	1:X:492:G:H5''	2.33	0.44
3:A:209:ALA:C	3:A:211:ARG:H	2.21	0.44
3:A:43:ARG:HG3	3:A:54:ILE:O	2.18	0.44
10:H:24:VAL:HG13	10:H:45:ALA:HB2	1.99	0.44
12:J:78:LYS:HE2	12:J:81:GLU:HA	2.00	0.44
18:P:72:LEU:HD12	18:P:126:ILE:HD13	2.00	0.44
11:I:8:PRO:HB2	11:I:14:LYS:NZ	2.32	0.44
14:L:8:ARG:CG	14:L:9:ARG:H	2.31	0.44
19:Q:51:ILE:HD11	19:Q:81:ARG:HD3	2.00	0.44
21:S:3:LEU:HB3	21:S:34:LEU:HB3	1.99	0.44
1:X:2506:C:H5'	30:4:33:LYS:HD2	2.00	0.43
5:C:107:ALA:HB1	5:C:180:ILE:HD11	2.00	0.43
19:Q:39:LYS:HG2	19:Q:43:GLN:HE21	1.83	0.43
1:X:1101:U:H2'	1:X:1102:G:C8	2.53	0.43
1:X:2506:C:H5''	30:4:30:VAL:HB	2.00	0.43
3:A:247:VAL:CG2	3:A:248:THR:N	2.81	0.43
5:C:150:LEU:HA	5:C:187:VAL:HB	2.00	0.43
5:C:95:LEU:CD2	5:C:96:PRO:HD2	2.48	0.43
9:G:43:VAL:HB	9:G:167:LYS:HG2	1.99	0.43
13:K:34:ILE:HG13	13:K:113:ILE:HG23	2.01	0.43
21:S:117:VAL:HG23	21:S:168:VAL:HG13	2.00	0.43
1:X:1230:C:H2'	1:X:1231:A:H8	1.83	0.43
1:X:1333:G:N7	1:X:1342:U:H5'	2.32	0.43
1:X:2324:G:H5''	1:X:2326:C:O4'	2.18	0.43
1:X:760:U:C6	26:Z:3:LYS:HG3	2.53	0.43
3:A:145:LEU:HB3	3:A:155:LEU:HD12	2.00	0.43
3:A:202:LYS:C	3:A:204:ILE:H	2.22	0.43
4:B:134:TRP:CD1	4:B:134:TRP:N	2.76	0.43
6:D:117:ILE:HD13	6:D:130:LEU:HD11	2.00	0.43
11:I:54:SER:HA	11:I:58:ALA:HB3	2.00	0.43
1:X:114:C:H2'	1:X:115:G:C8	2.53	0.43
1:X:2551:A:O5'	1:X:2553:G:H4'	2.18	0.43
5:C:127:ASP:HB2	5:C:128:ALA:H	1.64	0.43
1:X:342:G:O3'	1:X:343:A:C8	2.71	0.43
1:X:695:G:N2	1:X:808:C:O2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:4:HIS:HB3	26:Z:5:PRO:CD	2.45	0.43
5:C:133:PHE:HB2	5:C:160:ALA:HB1	2.00	0.43
5:C:30:VAL:HG11	5:C:177:VAL:HG21	2.00	0.43
1:X:538:A:H5''	9:G:139:ARG:HE	1.83	0.43
12:J:62:GLY:H	21:S:175:ARG:N	2.16	0.43
1:X:1577:G:H2'	1:X:1578:U:O4'	2.19	0.43
1:X:1996:A:H5'	18:P:118:LYS:NZ	2.33	0.43
1:X:2594:U:H2'	1:X:2595:C:H6	1.83	0.43
32:X:2929:1F4:C41	32:X:2929:1F4:C16	2.97	0.43
1:X:314:G:H2'	1:X:315:G:C8	2.53	0.43
1:X:84:G:N3	1:X:101:A:C2	2.86	0.43
2:Y:91:A:H2'	2:Y:92:G:C8	2.54	0.43
30:4:19:ARG:HD2	30:4:24:LEU:HD22	2.01	0.43
1:X:1782:A:O3'	3:A:206:LEU:HB2	2.18	0.43
3:A:245:VAL:N	3:A:252:LYS:HE3	2.34	0.43
5:C:170:LEU:HA	5:C:171:PRO:HD3	1.95	0.43
5:C:74:VAL:O	5:C:77:PHE:HB2	2.18	0.43
10:H:22:ILE:HD11	10:H:54:SER:HB2	1.99	0.43
17:O:69:ILE:HG22	17:O:86:HIS:HB3	2.00	0.43
1:X:339:U:H4'	20:R:77:HIS:ND1	2.34	0.43
1:X:1539:U:H2'	1:X:1540:C:C6	2.54	0.43
1:X:2006:G:H4'	1:X:2596:C:O3'	2.19	0.43
1:X:2066:G:N2	1:X:2216:G:H1'	2.34	0.43
1:X:2170:C:H2'	1:X:2171:U:H4'	2.01	0.43
1:X:2277:A:H2'	1:X:2278:A:O4'	2.18	0.43
3:A:63:ARG:O	3:A:65:ILE:HD12	2.18	0.43
18:P:25:PHE:C	18:P:25:PHE:CD2	2.90	0.43
12:J:61:ARG:HD3	21:S:174:PRO:HB2	1.99	0.43
1:X:1919:A:C2	1:X:1926:U:N3	2.74	0.43
1:X:2825:A:H2'	1:X:2826:C:C6	2.54	0.43
1:X:742:G:N1	3:A:208:LYS:HD3	2.33	0.43
3:A:45:ASN:CG	3:A:46:ARG:N	2.72	0.43
10:H:19:ILE:HG22	10:H:55:VAL:HA	2.01	0.43
10:H:27:SER:OG	10:H:49:ASP:HA	2.19	0.43
15:M:22:ARG:HD2	15:M:83:PHE:O	2.19	0.43
1:X:1148:G:O2'	9:G:134:MET:HG3	2.18	0.43
1:X:1283:C:H5''	1:X:1284:G:O5'	2.19	0.43
4:B:11:MET:HA	4:B:23:VAL:O	2.19	0.43
5:C:148:VAL:O	5:C:167:VAL:HA	2.19	0.43
10:H:10:VAL:HG11	10:H:98:ILE:HD12	2.00	0.43
13:K:33:ARG:HD3	13:K:112:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:66:ASN:HB3	16:N:76:TYR:N	2.27	0.43
20:R:24:VAL:HB	20:R:29:HIS:O	2.19	0.43
1:X:1469:U:OP1	1:X:1471:G:OP2	2.36	0.43
1:X:1643:A:H61	1:X:1656:U:H3	1.67	0.43
1:X:205:A:C8	1:X:205:A:H3'	2.54	0.43
1:X:2320:G:H2'	1:X:2321:C:O4'	2.19	0.43
32:X:2929:1F4:H53	32:X:2929:1F4:H9	2.00	0.43
1:X:551:A:H2'	1:X:552:C:O4'	2.19	0.43
1:X:1268:U:H5	5:C:68:ARG:HB2	1.84	0.43
1:X:504:G:N2	18:P:78:ASN:HD21	2.17	0.43
20:R:18:LYS:HD3	20:R:18:LYS:H	1.84	0.43
25:W:27:LYS:O	25:W:30:ASP:HB2	2.19	0.43
1:X:1497:C:H5''	1:X:1497:C:H6	1.84	0.43
1:X:882:C:H2'	1:X:883:A:O4'	2.19	0.43
2:Y:107:C:H2'	2:Y:108:G:O4'	2.19	0.43
2:Y:32:C:H1'	2:Y:59:A:H61	1.84	0.43
3:A:201:HIS:CD2	3:A:204:ILE:HD12	2.54	0.42
5:C:130:THR:HG23	5:C:160:ALA:HA	2.00	0.42
7:E:33:LEU:HD13	7:E:136:ILE:HG22	2.01	0.42
9:G:45:ASP:HA	9:G:83:ILE:HG13	2.01	0.42
13:K:90:ARG:HA	13:K:91:PRO:HD3	1.89	0.42
21:S:149:ALA:HB3	21:S:164:PRO:HA	1.99	0.42
1:X:1373:G:H22	1:X:2192:U:H3	1.67	0.42
1:X:1978:U:H3'	1:X:1979:C:H2'	2.01	0.42
1:X:2235:G:N2	1:X:2254:C:C4	2.87	0.42
1:X:487:G:H4'	1:X:512:A:N1	2.34	0.42
7:E:6:LYS:H	7:E:65:HIS:HE1	1.66	0.42
25:W:12:ARG:CG	25:W:12:ARG:NH1	2.76	0.42
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.52	0.42
1:X:322:A:H3'	1:X:323:G:H8	1.83	0.42
1:X:636:G:H8	1:X:636:G:H5''	1.84	0.42
1:X:719:A:H2'	1:X:720:A:O4'	2.19	0.42
26:Z:6:VAL:HG22	26:Z:7:PRO:HD2	2.00	0.42
7:E:126:PRO:HG2	7:E:130:ARG:HH22	1.85	0.42
18:P:46:ARG:HG3	18:P:95:ALA:HB3	2.01	0.42
20:R:93:ARG:HG2	20:R:108:VAL:HA	2.01	0.42
1:X:1371:G:H8	1:X:1371:G:O5'	2.02	0.42
1:X:2011:U:H2'	1:X:2012:A:O4'	2.19	0.42
1:X:2024:U:H2'	1:X:2025:A:O4'	2.20	0.42
1:X:2220:A:H2'	1:X:2221:G:C8	2.54	0.42
1:X:2489:C:C4	1:X:2490:U:C5	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:5:A:H2'	1:X:6:A:C8	2.54	0.42
1:X:812:G:H3'	1:X:813:A:H2'	2.01	0.42
10:H:64:VAL:HG22	10:H:106:ARG:NH1	2.35	0.42
1:X:638:A:C8	11:I:74:VAL:HG11	2.55	0.42
15:M:34:ARG:HH22	15:M:90:GLN:N	2.17	0.42
2:Y:108:G:H4'	21:S:26:LYS:HB3	2.02	0.42
1:X:2427:A:HO2'	1:X:2428:U:H5	1.64	0.42
1:X:346:C:O2	1:X:347:C:C5	2.72	0.42
1:X:441:A:H3'	1:X:442:A:H8	1.84	0.42
5:C:122:GLY:C	5:C:124:ASP:H	2.22	0.42
5:C:117:LEU:HD23	5:C:187:VAL:HG22	2.01	0.42
14:L:44:ASP:HB2	14:L:51:LEU:HD13	2.01	0.42
1:X:1656:U:C2'	1:X:1657:A:H5''	2.50	0.42
1:X:2200:G:H2'	1:X:2201:G:C8	2.55	0.42
1:X:877:G:H2'	1:X:878:C:C6	2.55	0.42
1:X:958:G:H2'	1:X:959:C:H6	1.84	0.42
2:Y:91:A:H8	2:Y:91:A:OP2	2.03	0.42
3:A:43:ARG:HD2	3:A:43:ARG:H	1.78	0.42
4:B:16:LYS:HB2	4:B:21:ILE:CD1	2.49	0.42
11:I:119:THR:HG23	11:I:139:ARG:HB3	2.02	0.42
1:X:1332:G:C6	1:X:1333:G:N1	2.88	0.42
1:X:2683:C:H2'	1:X:2684:A:O4'	2.19	0.42
1:X:50:G:H4'	1:X:51:A:H5'	2.02	0.42
1:X:700:C:H2'	1:X:701:U:O4'	2.20	0.42
4:B:131:SER:HB3	4:B:134:TRP:HD1	1.79	0.42
1:X:2658:A:H4'	4:B:165:VAL:HG11	2.02	0.42
4:B:152:LYS:N	9:G:106:TYR:HB3	2.33	0.42
1:X:2545:A:H61	10:H:40:GLY:CA	2.32	0.42
16:N:13:ARG:HA	16:N:16:LYS:HE2	2.02	0.42
17:O:12:TYR:HB2	17:O:40:VAL:H	1.84	0.42
17:O:88:GLN:HE21	17:O:88:GLN:HA	1.85	0.42
1:X:1737:G:H2'	1:X:1738:U:C6	2.55	0.42
1:X:205:A:H8	1:X:205:A:H3'	1.84	0.42
1:X:810:U:H2'	1:X:811:G:O4'	2.20	0.42
2:Y:102:A:H2'	2:Y:103:A:C8	2.54	0.42
2:Y:89:G:H5''	2:Y:90:C:OP2	2.19	0.42
3:A:173:VAL:HG23	3:A:187:SER:HB3	2.02	0.42
11:I:82:ASP:H	11:I:114:ILE:HG21	1.84	0.42
14:L:68:ALA:HB1	14:L:102:ALA:HB3	2.01	0.42
19:Q:62:ARG:O	19:Q:70:GLY:HA3	2.19	0.42
1:X:2241:U:C5	22:T:17:ASN:OD1	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:22:GLY:HA3	23:U:39:LYS:CD	2.49	0.42
1:X:1381:G:H8	1:X:1381:G:O5'	2.03	0.42
1:X:1279:G:O2'	1:X:1995:G:O6	2.26	0.42
1:X:2352:A:H2'	1:X:2353:G:C8	2.54	0.42
1:X:2528:G:H2'	1:X:2529:G:C8	2.49	0.42
1:X:2687:G:H2'	1:X:2688:G:H8	1.85	0.42
1:X:590:C:H2'	1:X:591:G:C8	2.55	0.42
5:C:194:GLU:O	5:C:195:ILE:HG12	2.20	0.42
5:C:33:TRP:CE3	5:C:95:LEU:HD12	2.54	0.42
9:G:157:PRO:C	9:G:159:SER:H	2.23	0.42
4:B:193:GLY:O	15:M:2:GLN:N	2.53	0.42
23:U:31:GLY:HA2	23:U:32:ARG:HH11	1.85	0.42
1:X:1035:G:C8	1:X:1036:G:H2'	2.55	0.42
1:X:1100:G:H21	1:X:1113:C:H42	1.67	0.42
1:X:1314:A:H2	1:X:1642:G:N3	2.17	0.42
1:X:1765:C:O5'	1:X:1765:C:H6	2.03	0.42
1:X:1774:A:C6	1:X:2566:A:C2	3.08	0.42
1:X:1804:U:H2'	1:X:1805:G:C8	2.54	0.42
1:X:631:G:H4'	1:X:632:A:H5'	2.02	0.42
1:X:666:U:O2'	1:X:667:U:H5''	2.20	0.42
1:X:688:A:N3	1:X:2422:C:O2'	2.46	0.42
1:X:708:G:OP1	1:X:1393:G:O2'	2.37	0.42
5:C:180:ILE:HG13	5:C:181:LEU:N	2.35	0.42
9:G:170:PRO:HB2	9:G:171:LEU:H	1.75	0.42
15:M:38:LYS:HB3	15:M:46:ARG:HB3	2.01	0.42
1:X:1447:U:HO2'	1:X:1448:A:H8	1.65	0.42
1:X:1929:U:H2'	1:X:1930:C:C6	2.54	0.42
5:C:94:THR:HG22	5:C:100:ARG:HH12	1.84	0.41
9:G:132:PHE:HZ	9:G:142:ARG:HA	1.85	0.41
10:H:132:GLU:HG2	10:H:134:LEU:HG	2.02	0.41
11:I:28:LYS:HZ1	11:I:36:GLY:HA2	1.83	0.41
13:K:76:VAL:O	13:K:80:MET:HB2	2.20	0.41
13:K:8:ARG:O	13:K:9:LYS:HB3	2.20	0.41
1:X:1167:A:C5	16:N:51:ARG:HD3	2.55	0.41
20:R:29:HIS:CD2	20:R:51:VAL:HG22	2.55	0.41
1:X:1302:C:H2'	1:X:1303:U:H6	1.85	0.41
1:X:149:A:H2'	1:X:150:A:H8	1.84	0.41
1:X:554:U:H4'	1:X:555:U:OP2	2.20	0.41
24:V:32:ALA:HB2	24:V:37:LEU:HG	2.02	0.41
1:X:1975:G:N2	1:X:1979:C:O2'	2.52	0.41
1:X:2053:G:H2'	1:X:2054:A:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:224:G:H4'	1:X:399:G:C4	2.55	0.41
1:X:2796:A:H2'	1:X:2797:G:C8	2.55	0.41
32:X:2929:1F4:H18	32:X:2929:1F4:C53	2.50	0.41
1:X:54:G:C2	1:X:114:C:C2	3.08	0.41
1:X:622:U:H2'	1:X:623:G:O4'	2.21	0.41
12:J:6:LYS:O	12:J:71:PRO:HD2	2.20	0.41
23:U:47:HIS:HB2	23:U:48:LYS:H	1.71	0.41
1:X:1032:A:C3'	1:X:1032:A:C8	3.03	0.41
1:X:1249:G:O2'	1:X:1250:A:H8	2.03	0.41
1:X:1385:C:H2'	1:X:1386:A:O4'	2.20	0.41
1:X:1287:A:H2	1:X:1661:C:O2	2.03	0.41
1:X:1973:C:H2'	1:X:1974:U:O4'	2.21	0.41
1:X:692:C:H2'	1:X:693:A:C8	2.55	0.41
1:X:2859:U:N3	26:Z:52:TYR:CE1	2.88	0.41
1:X:1811:A:H3'	3:A:178:PRO:HB2	2.02	0.41
1:X:1266:G:C8	11:I:32:ARG:NH1	2.85	0.41
11:I:60:LEU:HA	11:I:60:LEU:HD12	1.89	0.41
12:J:64:LYS:HG2	21:S:112:LEU:HD22	2.02	0.41
25:W:4:LYS:HE3	25:W:52:GLU:O	2.20	0.41
1:X:2209:G:H4'	23:U:46:LEU:HB2	2.02	0.41
1:X:237:G:H1'	1:X:632:A:H1'	2.02	0.41
1:X:649:G:H2'	1:X:650:U:C6	2.55	0.41
1:X:934:G:H1'	22:T:26:PHE:CD1	2.55	0.41
1:X:960:U:H2'	1:X:961:G:H8	1.82	0.41
6:D:75:SER:HB2	6:D:79:LEU:HB2	2.03	0.41
12:J:36:ILE:HG13	12:J:103:VAL:HA	2.03	0.41
12:J:6:LYS:HE3	12:J:7:ARG:HE	1.86	0.41
1:X:1224:A:H4'	1:X:1225:G:OP2	2.20	0.41
1:X:1381:G:H2'	1:X:1799:A:H61	1.86	0.41
1:X:1687:C:H6	1:X:1687:C:O5'	2.02	0.41
4:B:104:ALA:HB3	4:B:170:LEU:HD12	2.02	0.41
11:I:28:LYS:HZ3	11:I:36:GLY:HA2	1.86	0.41
13:K:96:ARG:O	13:K:113:ILE:HA	2.20	0.41
23:U:65:ASN:N	23:U:65:ASN:OD1	2.54	0.41
1:X:1792:C:N4	1:X:2185:U:H5'	2.36	0.41
1:X:2225:G:H2'	1:X:2226:A:H8	1.85	0.41
1:X:2556:A:H5''	1:X:2557:G:H5'	2.02	0.41
1:X:2590:U:O4'	32:X:2929:1F4:H32	2.21	0.41
3:A:213:ARG:HD2	3:A:213:ARG:HA	1.97	0.41
5:C:171:PRO:O	5:C:173:ALA:N	2.54	0.41
9:G:62:ILE:HG23	9:G:135:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:34:ARG:NH1	15:M:91:VAL:HB	2.36	0.41
21:S:141:MET:SD	21:S:147:ILE:HG12	2.61	0.41
1:X:1117:G:H2'	1:X:1118:G:C8	2.55	0.41
1:X:1:G:H2'	1:X:1:G:N3	2.36	0.41
1:X:2633:A:N1	1:X:2644:A:H5''	2.35	0.41
1:X:2519:C:O2'	1:X:2720:A:N3	2.44	0.41
1:X:946:U:H2'	1:X:947:C:C6	2.56	0.41
9:G:53:ARG:HH22	9:G:171:LEU:HD12	1.85	0.41
12:J:14:PHE:CE1	12:J:90:ALA:HB2	2.56	0.41
1:X:1132:C:H6	1:X:1132:C:O5'	2.03	0.41
1:X:2395:C:H2'	1:X:2396:C:H5''	2.02	0.41
1:X:654:A:C2	1:X:655:A:H3'	2.56	0.41
4:B:105:THR:HB	4:B:166:THR:HG23	2.03	0.41
12:J:27:TYR:HB2	12:J:137:VAL:HG21	2.02	0.41
14:L:31:VAL:HG23	14:L:38:ILE:HD11	2.01	0.41
16:N:68:GLY:HA2	16:N:71:LEU:HD23	2.02	0.41
20:R:22:VAL:HG22	20:R:83:LEU:H	1.85	0.41
21:S:107:GLU:HG3	21:S:112:LEU:HA	2.02	0.41
23:U:14:VAL:HB	23:U:15:VAL:H	1.75	0.41
1:X:322:A:H3'	1:X:323:G:C8	2.55	0.41
4:B:55:ALA:HB3	4:B:58:LYS:HD2	2.01	0.41
7:E:24:PHE:HB2	7:E:37:TYR:HD1	1.85	0.41
1:X:494:A:C8	20:R:56:LYS:HD2	2.56	0.41
1:X:95:G:H4'	24:V:41:HIS:ND1	2.35	0.41
1:X:1009:C:H2'	1:X:1010:U:O4'	2.21	0.41
1:X:1106:A:H2'	1:X:1107:A:H8	1.86	0.41
1:X:762:A:H4'	1:X:1284:G:N3	2.36	0.41
5:C:176:ASN:ND2	5:C:179:ASP:H	2.16	0.41
14:L:76:ALA:HB2	14:L:107:ALA:HA	2.02	0.41
1:X:2357:A:H1'	14:L:88:VAL:HG11	2.02	0.41
17:O:19:VAL:HG13	17:O:90:PHE:CD1	2.56	0.41
1:X:1615:C:OP2	19:Q:35:LYS:HD2	2.20	0.41
22:T:38:VAL:CG1	22:T:59:LEU:HD12	2.50	0.41
1:X:1467:U:H3'	1:X:1467:U:H6	1.85	0.41
1:X:1469:U:H5'	1:X:1470:G:N7	2.36	0.41
1:X:1533:G:H2'	1:X:1534:A:H8	1.86	0.41
1:X:1494:G:HO2'	1:X:1574:A:H2	1.66	0.41
1:X:188:G:H2'	1:X:189:A:C8	2.56	0.41
1:X:657:A:C8	1:X:657:A:H3'	2.56	0.41
1:X:874:A:H2'	1:X:875:G:O4'	2.21	0.41
1:X:98:U:H1'	1:X:100:G:C4	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:14:LYS:CA	28:2:15:THR:CA	2.98	0.40
5:C:30:VAL:HA	5:C:95:LEU:HD11	2.02	0.40
16:N:88:ILE:HG13	17:O:49:GLU:HB2	2.03	0.40
18:P:19:LYS:HB3	18:P:19:LYS:HE2	1.76	0.40
24:V:2:LYS:H	24:V:3:PRO:CD	2.33	0.40
1:X:99:U:H5''	1:X:100:G:C8	2.57	0.40
1:X:1835:C:H2'	1:X:1836:C:C6	2.56	0.40
1:X:2526:U:H2'	1:X:2527:G:C8	2.57	0.40
1:X:956:A:C5	1:X:2427:A:C2	3.09	0.40
3:A:147:LEU:HD22	3:A:183:ARG:NH2	2.35	0.40
1:X:1835:C:O2'	3:A:254:THR:HB	2.21	0.40
19:Q:56:MET:SD	19:Q:57:ASN:N	2.91	0.40
21:S:53:ASP:HA	21:S:63:PRO:HA	2.03	0.40
22:T:41:ARG:HA	22:T:41:ARG:NE	2.34	0.40
23:U:43:ARG:HH21	23:U:43:ARG:HB2	1.85	0.40
1:X:1248:G:O5'	1:X:1248:G:H8	2.04	0.40
1:X:2796:A:OP2	13:K:5:LYS:NZ	2.55	0.40
1:X:957:G:H2'	1:X:958:G:H8	1.86	0.40
3:A:166:GLN:HB2	3:A:174:ILE:HG22	2.03	0.40
3:A:202:LYS:C	3:A:204:ILE:N	2.75	0.40
12:J:70:PHE:HA	12:J:71:PRO:HD3	1.95	0.40
16:N:42:ALA:O	16:N:46:GLU:N	2.51	0.40
23:U:20:ARG:HB2	23:U:43:ARG:HD2	2.02	0.40
1:X:2064:U:H2'	1:X:2065:A:C8	2.56	0.40
1:X:2419:C:N3	1:X:2420:C:H1'	2.37	0.40
32:X:2929:1F4:O46	32:X:2929:1F4:H7	2.22	0.40
1:X:651:C:H2'	1:X:652:C:H6	1.86	0.40
1:X:649:G:N2	1:X:660:G:N2	2.69	0.40
2:Y:22:U:H3	2:Y:65:A:H61	1.68	0.40
26:Z:36:CYS:HB3	26:Z:49:CYS:HB3	1.94	0.40
26:Z:42:SER:O	26:Z:44:HIS:HD2	2.03	0.40
1:X:1796:A:N3	3:A:50:THR:HG23	2.36	0.40
1:X:506:G:H4'	18:P:21:ARG:HH21	1.85	0.40
21:S:36:ARG:O	21:S:40:ASP:HB2	2.22	0.40
1:X:1519:G:H2'	1:X:1520:G:H8	1.86	0.40
1:X:877:G:H2'	1:X:878:C:H6	1.86	0.40
7:E:140:LEU:O	7:E:144:VAL:HG23	2.22	0.40
9:G:103:TYR:HB3	9:G:107:GLN:HE21	1.85	0.40
4:B:181:LEU:HD21	15:M:12:LEU:CD2	2.51	0.40
16:N:95:LEU:HA	16:N:98:ILE:HD12	2.04	0.40
17:O:10:LYS:HE3	17:O:11:GLN:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1255:A:H2'	1:X:1256:C:H6	1.86	0.40
1:X:1467:U:H5''	1:X:1467:U:C6	2.57	0.40
1:X:2042:A:O3'	5:C:63:GLY:HA2	2.21	0.40
1:X:2422:C:H2'	1:X:2423:G:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	238/274 (87%)	173 (73%)	47 (20%)	18 (8%)	1	12
4	B	203/211 (96%)	173 (85%)	25 (12%)	5 (2%)	5	36
5	C	195/205 (95%)	127 (65%)	40 (20%)	28 (14%)	0	4
6	D	175/180 (97%)	142 (81%)	26 (15%)	7 (4%)	3	26
7	E	169/185 (91%)	134 (79%)	26 (15%)	9 (5%)	2	19
8	F	69/144 (48%)	57 (83%)	9 (13%)	3 (4%)	2	24
9	G	140/174 (80%)	99 (71%)	26 (19%)	15 (11%)	0	7
10	H	132/134 (98%)	117 (89%)	12 (9%)	3 (2%)	6	38
11	I	139/156 (89%)	81 (58%)	39 (28%)	19 (14%)	0	4
12	J	134/141 (95%)	98 (73%)	24 (18%)	12 (9%)	1	9
13	K	111/116 (96%)	92 (83%)	13 (12%)	6 (5%)	2	19
14	L	102/114 (90%)	75 (74%)	15 (15%)	12 (12%)	0	5
15	M	106/166 (64%)	90 (85%)	10 (9%)	6 (6%)	1	18
16	N	115/118 (98%)	91 (79%)	17 (15%)	7 (6%)	1	17
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	4
18	P	125/134 (93%)	104 (83%)	17 (14%)	4 (3%)	4	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Q	91/95 (96%)	63 (69%)	16 (18%)	12 (13%)	0	4
20	R	108/115 (94%)	65 (60%)	26 (24%)	17 (16%)	0	3
21	S	173/237 (73%)	135 (78%)	27 (16%)	11 (6%)	1	17
22	T	82/91 (90%)	65 (79%)	12 (15%)	5 (6%)	1	17
23	U	70/81 (86%)	41 (59%)	15 (21%)	14 (20%)	0	1
24	V	64/67 (96%)	57 (89%)	5 (8%)	2 (3%)	4	32
25	W	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	8	42
26	Z	56/60 (93%)	45 (80%)	6 (11%)	5 (9%)	1	9
30	4	35/37 (95%)	23 (66%)	11 (31%)	1 (3%)	4	33
All	All	2977/3390 (88%)	2260 (76%)	482 (16%)	235 (8%)	1	11

All (235) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	45	ASN
3	A	209	ALA
3	A	217	ARG
3	A	248	THR
3	A	249	PRO
3	A	250	TRP
3	A	271	VAL
5	C	4	ILE
5	C	20	PRO
5	C	60	GLY
5	C	66	ASN
5	C	129	LYS
5	C	164	VAL
5	C	165	SER
5	C	172	VAL
5	C	195	ILE
6	D	10	ASP
6	D	81	GLN
6	D	122	PHE
7	E	165	VAL
9	G	33	ILE
9	G	67	ARG
9	G	92	GLY
9	G	97	ASP
9	G	104	THR

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Mol	Chain	Res	Type
9	G	170	PRO
10	H	27	SER
11	I	18	ARG
11	I	47	ALA
11	I	49	PHE
11	I	64	GLY
11	I	98	LEU
11	I	99	VAL
11	I	103	ASN
12	J	80	ALA
12	J	82	THR
12	J	88	LYS
13	K	6	ALA
13	K	92	GLY
14	L	21	THR
14	L	61	SER
14	L	68	ALA
14	L	95	LYS
15	M	29	PRO
16	N	8	ILE
16	N	95	LEU
17	O	7	THR
17	O	10	LYS
17	O	22	VAL
17	O	48	GLY
19	Q	6	ILE
19	Q	61	LYS
19	Q	63	LYS
19	Q	67	ARG
19	Q	69	ILE
20	R	11	ASN
20	R	15	HIS
20	R	60	PRO
20	R	82	ALA
20	R	107	ALA
21	S	6	LYS
21	S	26	LYS
21	S	56	VAL
21	S	91	PRO
21	S	156	GLU
22	T	19	LYS
23	U	15	VAL

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Mol	Chain	Res	Type
23	U	19	ILE
23	U	32	ARG
23	U	34	THR
23	U	56	GLN
23	U	60	VAL
26	Z	4	HIS
26	Z	36	CYS
26	Z	53	ASP
3	A	35	GLU
3	A	58	HIS
3	A	220	HIS
4	B	132	LYS
5	C	22	VAL
5	C	83	ALA
5	C	121	ASP
5	C	190	ALA
5	C	196	VAL
6	D	124	GLY
7	E	59	GLN
7	E	173	ALA
9	G	37	ASP
9	G	105	GLY
9	G	107	GLN
9	G	158	HIS
10	H	5	GLN
10	H	29	ILE
11	I	36	GLY
11	I	54	SER
11	I	62	LYS
11	I	68	VAL
12	J	11	ARG
12	J	83	ARG
12	J	87	GLY
12	J	91	VAL
13	K	4	GLY
13	K	9	LYS
14	L	31	VAL
14	L	40	ALA
14	L	94	TYR
15	M	26	ASP
15	M	31	ASP
15	M	39	VAL

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Mol	Chain	Res	Type
15	M	57	ILE
16	N	7	GLY
16	N	87	ASN
17	O	8	GLY
17	O	9	GLY
17	O	14	VAL
18	P	9	ARG
18	P	85	MET
19	Q	12	ILE
19	Q	84	GLU
20	R	85	ASP
20	R	98	ILE
22	T	11	LYS
23	U	29	GLY
23	U	41	VAL
23	U	76	LYS
24	V	2	LYS
24	V	36	GLN
30	4	3	VAL
3	A	254	THR
3	A	269	PHE
4	B	129	HIS
4	B	146	THR
5	C	9	GLN
5	C	10	ASN
5	C	15	ILE
5	C	67	ALA
5	C	113	GLU
5	C	114	GLY
5	C	163	ASN
5	C	189	ASP
6	D	71	LYS
6	D	119	PRO
9	G	34	PRO
11	I	91	ASP
12	J	81	GLU
14	L	33	ARG
14	L	52	ALA
15	M	74	GLY
16	N	92	ARG
16	N	94	VAL
17	O	11	GLN

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Mol	Chain	Res	Type
17	O	49	GLU
18	P	132	GLY
19	Q	62	ARG
19	Q	74	ASP
19	Q	89	GLU
20	R	14	LEU
20	R	83	LEU
20	R	87	GLU
20	R	96	LYS
21	S	88	TYR
21	S	128	ARG
22	T	74	LYS
23	U	27	ASP
26	Z	24	ALA
26	Z	37	HIS
3	A	54	ILE
3	A	55	GLY
5	C	13	ARG
5	C	18	PRO
5	C	194	GLU
6	D	40	LEU
7	E	19	ALA
7	E	65	HIS
8	F	118	GLY
9	G	159	SER
11	I	59	ARG
11	I	65	PHE
11	I	90	ARG
12	J	17	ARG
12	J	29	ALA
13	K	95	THR
14	L	60	LYS
17	O	31	ASP
17	O	36	LYS
17	O	78	VAL
19	Q	87	SER
20	R	63	THR
21	S	33	ALA
21	S	74	ARG
22	T	13	GLY
22	T	27	GLY
3	A	247	VAL

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Mol	Chain	Res	Type
3	A	255	LYS
4	B	90	SER
5	C	55	GLY
5	C	68	ARG
7	E	7	GLN
7	E	55	PRO
7	E	92	VAL
11	I	37	GLN
11	I	115	SER
12	J	21	ASP
14	L	53	ALA
17	O	30	GLY
20	R	6	ALA
20	R	108	VAL
23	U	26	ALA
23	U	47	HIS
25	W	14	GLY
3	A	187	SER
4	B	137	ARG
5	C	126	ALA
9	G	165	VAL
11	I	86	THR
13	K	93	GLY
14	L	39	TYR
16	N	65	ILE
18	P	20	LEU
20	R	50	GLY
21	S	125	PRO
23	U	12	ASN
9	G	68	PRO
12	J	28	VAL
20	R	51	VAL
7	E	126	PRO
8	F	96	VAL
11	I	9	THR
21	S	174	PRO
8	F	120	VAL
20	R	111	GLY
3	A	270	ILE
9	G	138	GLY
19	Q	66	GLY
23	U	14	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	185/215 (86%)	145 (78%)	40 (22%)	1	6
4	B	155/157 (99%)	119 (77%)	36 (23%)	1	5
5	C	157/163 (96%)	112 (71%)	45 (29%)	0	3
6	D	153/156 (98%)	130 (85%)	23 (15%)	3	19
7	E	136/144 (94%)	115 (85%)	21 (15%)	2	18
8	F	51/107 (48%)	49 (96%)	2 (4%)	32	65
9	G	118/146 (81%)	94 (80%)	24 (20%)	1	8
10	H	103/103 (100%)	80 (78%)	23 (22%)	1	6
11	I	108/121 (89%)	79 (73%)	29 (27%)	0	3
12	J	110/115 (96%)	89 (81%)	21 (19%)	1	9
13	K	90/93 (97%)	76 (84%)	14 (16%)	2	18
14	L	74/82 (90%)	51 (69%)	23 (31%)	0	2
15	M	94/134 (70%)	71 (76%)	23 (24%)	0	4
16	N	96/97 (99%)	76 (79%)	20 (21%)	1	7
17	O	75/79 (95%)	56 (75%)	19 (25%)	0	4
18	P	109/115 (95%)	91 (84%)	18 (16%)	2	15
19	Q	75/76 (99%)	60 (80%)	15 (20%)	1	8
20	R	91/96 (95%)	75 (82%)	16 (18%)	2	12
21	S	149/192 (78%)	117 (78%)	32 (22%)	1	6
22	T	62/67 (92%)	53 (86%)	9 (14%)	3	20
23	U	57/66 (86%)	33 (58%)	24 (42%)	0	0
24	V	54/55 (98%)	43 (80%)	11 (20%)	1	8
25	W	48/48 (100%)	37 (77%)	11 (23%)	1	5
26	Z	51/53 (96%)	41 (80%)	10 (20%)	1	8
30	4	35/35 (100%)	29 (83%)	6 (17%)	2	13
All	All	2436/2715 (90%)	1921 (79%)	515 (21%)	1	7

All (515) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	37	LEU
3	A	39	LYS
3	A	40	THR
3	A	43	ARG
3	A	46	ARG
3	A	48	ARG
3	A	49	ILE
3	A	52	ARG
3	A	63	ARG
3	A	68	LYS
3	A	69	ARG
3	A	88	ARG
3	A	96	HIS
3	A	105	ILE
3	A	111	LEU
3	A	118	ASN
3	A	131	LEU
3	A	145	LEU
3	A	157	ARG
3	A	162	SER
3	A	169	GLU
3	A	183	ARG
3	A	186	HIS
3	A	196	VAL
3	A	203	ASN
3	A	208	LYS
3	A	212	SER
3	A	218	LYS
3	A	222	ARG
3	A	226	MET
3	A	240	THR
3	A	244	ARG
3	A	245	VAL
3	A	247	VAL
3	A	248	THR
3	A	250	TRP
3	A	252	LYS
3	A	254	THR
3	A	259	THR
3	A	270	ILE
4	B	2	LYS
4	B	4	ILE

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Mol	Chain	Res	Type
4	B	5	LEU
4	B	14	ILE
4	B	27	LEU
4	B	34	VAL
4	B	35	GLN
4	B	37	LYS
4	B	41	THR
4	B	49	ILE
4	B	69	LYS
4	B	72	VAL
4	B	75	THR
4	B	103	ASP
4	B	107	THR
4	B	113	THR
4	B	119	ARG
4	B	131	SER
4	B	133	LYS
4	B	134	TRP
4	B	136	ARG
4	B	137	ARG
4	B	140	SER
4	B	141	ILE
4	B	145	LYS
4	B	149	ARG
4	B	150	VAL
4	B	152	LYS
4	B	154	LYS
4	B	162	MET
4	B	163	GLU
4	B	165	VAL
4	B	192	ASN
4	B	198	LEU
4	B	200	SER
4	B	203	LYS
5	C	3	GLN
5	C	7	ILE
5	C	10	ASN
5	C	13	ARG
5	C	14	THR
5	C	15	ILE
5	C	45	THR
5	C	48	ARG

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Mol	Chain	Res	Type
5	C	51	VAL
5	C	52	SER
5	C	53	LYS
5	C	59	TYR
5	C	64	THR
5	C	66	ASN
5	C	71	ASP
5	C	72	ARG
5	C	76	THR
5	C	89	ARG
5	C	91	TYR
5	C	94	THR
5	C	95	LEU
5	C	97	ARG
5	C	118	VAL
5	C	121	ASP
5	C	123	PHE
5	C	124	ASP
5	C	127	ASP
5	C	130	THR
5	C	134	ILE
5	C	136	TRP
5	C	138	LYS
5	C	140	ASN
5	C	143	ASP
5	C	148	VAL
5	C	151	VAL
5	C	153	ASP
5	C	154	ASP
5	C	162	ARG
5	C	164	VAL
5	C	166	TRP
5	C	175	VAL
5	C	180	ILE
5	C	181	LEU
5	C	188	ILE
5	C	194	GLU
6	D	11	GLN
6	D	33	LYS
6	D	40	LEU
6	D	45	GLU
6	D	57	LEU

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Mol	Chain	Res	Type
6	D	60	ILE
6	D	63	GLN
6	D	67	ILE
6	D	71	LYS
6	D	80	ARG
6	D	89	VAL
6	D	95	ARG
6	D	112	ARG
6	D	115	ARG
6	D	125	ARG
6	D	130	LEU
6	D	134	GLU
6	D	136	LEU
6	D	148	LYS
6	D	150	ARG
6	D	153	ASP
6	D	171	GLN
6	D	175	LEU
7	E	15	VAL
7	E	21	ASP
7	E	35	VAL
7	E	40	GLU
7	E	44	ARG
7	E	50	LEU
7	E	59	GLN
7	E	67	LEU
7	E	69	ARG
7	E	72	VAL
7	E	81	ASP
7	E	86	ASN
7	E	97	LYS
7	E	98	LEU
7	E	121	VAL
7	E	130	ARG
7	E	133	VAL
7	E	139	GLN
7	E	140	LEU
7	E	141	VAL
7	E	155	ASP
8	F	78	ILE
8	F	101	TRP
9	G	31	THR

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Mol	Chain	Res	Type
9	G	38	GLU
9	G	41	TRP
9	G	56	THR
9	G	61	ARG
9	G	62	ILE
9	G	63	ARG
9	G	70	PHE
9	G	75	ILE
9	G	91	THR
9	G	95	LEU
9	G	101	THR
9	G	102	ARG
9	G	104	THR
9	G	112	THR
9	G	113	GLU
9	G	116	ARG
9	G	122	HIS
9	G	132	PHE
9	G	137	LYS
9	G	145	HIS
9	G	154	GLU
9	G	165	VAL
9	G	168	THR
10	H	1	MET
10	H	7	ARG
10	H	9	ASP
10	H	10	VAL
10	H	23	ARG
10	H	29	ILE
10	H	41	ASN
10	H	57	ASP
10	H	83	ARG
10	H	85	ASP
10	H	88	THR
10	H	89	ILE
10	H	90	ARG
10	H	94	ASN
10	H	102	GLN
10	H	106	ARG
10	H	109	ARG
10	H	116	ARG
10	H	117	GLU

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Mol	Chain	Res	Type
10	H	119	ARG
10	H	124	MET
10	H	126	ILE
10	H	127	VAL
11	I	4	HIS
11	I	6	LEU
11	I	13	ARG
11	I	18	ARG
11	I	21	ARG
11	I	26	THR
11	I	29	THR
11	I	32	ARG
11	I	39	SER
11	I	40	ARG
11	I	45	LYS
11	I	50	GLU
11	I	53	ARG
11	I	56	LEU
11	I	57	ILE
11	I	60	LEU
11	I	62	LYS
11	I	65	PHE
11	I	77	LEU
11	I	78	SER
11	I	83	LEU
11	I	85	ASP
11	I	86	THR
11	I	93	LEU
11	I	98	LEU
11	I	99	VAL
11	I	101	ARG
11	I	108	LEU
11	I	142	LEU
12	J	7	ARG
12	J	8	THR
12	J	11	ARG
12	J	17	ARG
12	J	32	ASP
12	J	43	ILE
12	J	44	LYS
12	J	52	ARG
12	J	54	VAL

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Mol	Chain	Res	Type
12	J	64	LYS
12	J	73	LYS
12	J	81	GLU
12	J	93	TYR
12	J	94	TRP
12	J	95	VAL
12	J	120	ARG
12	J	126	LEU
12	J	129	GLN
12	J	131	LYS
12	J	134	LYS
12	J	140	GLU
13	K	8	ARG
13	K	10	LEU
13	K	11	ASN
13	K	12	ARG
13	K	17	ARG
13	K	28	LEU
13	K	51	LEU
13	K	60	LEU
13	K	73	LYS
13	K	83	VAL
13	K	94	TYR
13	K	99	ARG
13	K	109	THR
13	K	115	LEU
14	L	8	ARG
14	L	11	LEU
14	L	12	ARG
14	L	13	THR
14	L	15	ARG
14	L	18	ARG
14	L	31	VAL
14	L	33	ARG
14	L	36	LYS
14	L	37	HIS
14	L	43	ILE
14	L	64	LYS
14	L	66	ASP
14	L	67	THR
14	L	87	VAL
14	L	88	VAL

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Mol	Chain	Res	Type
14	L	89	PHE
14	L	90	ASP
14	L	91	ARG
14	L	93	SER
14	L	94	TYR
14	L	99	ARG
14	L	108	ARG
15	M	5	ILE
15	M	6	LYS
15	M	7	ILE
15	M	12	LEU
15	M	13	LEU
15	M	14	ARG
15	M	31	ASP
15	M	34	ARG
15	M	35	VAL
15	M	40	ARG
15	M	54	VAL
15	M	57	ILE
15	M	63	ARG
15	M	68	VAL
15	M	69	ARG
15	M	78	GLU
15	M	79	ARG
15	M	89	ASN
15	M	93	ILE
15	M	95	GLU
15	M	98	LYS
15	M	99	VAL
15	M	100	ARG
16	N	3	ARG
16	N	5	LYS
16	N	8	ILE
16	N	9	VAL
16	N	13	ARG
16	N	18	LEU
16	N	22	LYS
16	N	25	TRP
16	N	40	LEU
16	N	51	ARG
16	N	58	ARG
16	N	60	LEU

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Mol	Chain	Res	Type
16	N	71	LEU
16	N	88	ILE
16	N	90	LEU
16	N	92	ARG
16	N	93	LYS
16	N	95	LEU
16	N	102	GLU
16	N	111	ASP
17	O	13	ARG
17	O	18	ASP
17	O	20	ILE
17	O	21	ARG
17	O	22	VAL
17	O	25	LEU
17	O	26	GLN
17	O	28	GLU
17	O	39	PHE
17	O	40	VAL
17	O	46	VAL
17	O	47	PHE
17	O	50	ASP
17	O	56	VAL
17	O	62	GLU
17	O	69	ILE
17	O	76	SER
17	O	78	VAL
17	O	88	GLN
18	P	9	ARG
18	P	11	LYS
18	P	32	ARG
18	P	60	ILE
18	P	62	ARG
18	P	71	VAL
18	P	72	LEU
18	P	84	GLU
18	P	86	LEU
18	P	87	GLU
18	P	91	PHE
18	P	109	ARG
18	P	111	ARG
18	P	113	SER
18	P	118	LYS

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Mol	Chain	Res	Type
18	P	124	ILE
18	P	125	THR
18	P	126	ILE
19	Q	7	LEU
19	Q	12	ILE
19	Q	14	GLU
19	Q	26	SER
19	Q	38	ILE
19	Q	40	ASP
19	Q	42	ILE
19	Q	56	MET
19	Q	58	VAL
19	Q	63	LYS
19	Q	65	VAL
19	Q	67	ARG
19	Q	81	ARG
19	Q	82	LEU
19	Q	84	GLU
20	R	13	LYS
20	R	18	LYS
20	R	23	ILE
20	R	25	LEU
20	R	26	SER
20	R	80	LYS
20	R	81	VAL
20	R	87	GLU
20	R	88	THR
20	R	98	ILE
20	R	104	VAL
20	R	105	ARG
20	R	106	VAL
20	R	108	VAL
20	R	112	LYS
20	R	113	THR
21	S	2	GLU
21	S	13	LYS
21	S	14	LEU
21	S	15	ASP
21	S	22	VAL
21	S	24	TYR
21	S	26	LYS
21	S	41	ARG

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Mol	Chain	Res	Type
21	S	46	GLN
21	S	48	THR
21	S	51	LEU
21	S	53	ASP
21	S	54	ILE
21	S	65	LEU
21	S	66	VAL
21	S	67	LYS
21	S	71	MET
21	S	76	ARG
21	S	79	ILE
21	S	94	VAL
21	S	95	SER
21	S	113	VAL
21	S	120	LEU
21	S	128	ARG
21	S	132	GLN
21	S	133	GLU
21	S	139	THR
21	S	152	ILE
21	S	155	PRO
21	S	160	LEU
21	S	163	ASP
21	S	166	LEU
22	T	5	LYS
22	T	16	SER
22	T	17	ASN
22	T	41	ARG
22	T	46	LYS
22	T	49	GLN
22	T	62	LEU
22	T	64	ASP
22	T	85	GLN
23	U	8	THR
23	U	11	LYS
23	U	13	LEU
23	U	14	VAL
23	U	17	SER
23	U	19	ILE
23	U	20	ARG
23	U	23	LYS
23	U	32	ARG

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Mol	Chain	Res	Type
23	U	37	ILE
23	U	40	ARG
23	U	42	GLN
23	U	43	ARG
23	U	45	ASN
23	U	47	HIS
23	U	52	ARG
23	U	57	VAL
23	U	62	LEU
23	U	63	SER
23	U	65	ASN
23	U	70	LEU
23	U	75	TYR
23	U	78	ILE
23	U	79	GLU
24	V	6	MET
24	V	7	ARG
24	V	13	ASP
24	V	14	PHE
24	V	21	ARG
24	V	25	LEU
24	V	28	LEU
24	V	41	HIS
24	V	53	LEU
24	V	60	LEU
24	V	65	GLU
25	W	4	LYS
25	W	6	VAL
25	W	9	VAL
25	W	10	ILE
25	W	12	ARG
25	W	26	ARG
25	W	32	ARG
25	W	34	VAL
25	W	36	ASP
25	W	37	THR
25	W	46	THR
26	Z	3	LYS
26	Z	4	HIS
26	Z	6	VAL
26	Z	8	LYS
26	Z	14	SER

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Mol	Chain	Res	Type
26	Z	18	MET
26	Z	25	LEU
26	Z	35	GLN
26	Z	40	LYS
26	Z	57	VAL
30	4	2	LYS
30	4	9	LYS
30	4	14	CYS
30	4	17	VAL
30	4	25	VAL
30	4	30	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	76	ASN
3	A	118	ASN
3	A	201	HIS
3	A	231	HIS
4	B	129	HIS
4	B	180	ASN
5	C	61	GLN
5	C	66	ASN
5	C	98	GLN
5	C	140	ASN
5	C	176	ASN
6	D	63	GLN
6	D	129	ASN
7	E	18	ASN
7	E	59	GLN
7	E	65	HIS
7	E	86	ASN
9	G	73	ASN
9	G	76	GLN
10	H	41	ASN
11	I	34	HIS
11	I	37	GLN
12	J	46	ASN
12	J	129	GLN
13	K	13	ASN
14	L	41	GLN
14	L	49	GLN

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Mol	Chain	Res	Type
15	M	58	ASN
15	M	90	GLN
16	N	31	GLN
16	N	66	ASN
16	N	75	ASN
17	O	6	GLN
17	O	11	GLN
17	O	79	GLN
17	O	88	GLN
18	P	78	ASN
18	P	81	HIS
18	P	115	ASN
19	Q	43	GLN
19	Q	44	GLN
19	Q	57	ASN
20	R	10	HIS
20	R	15	HIS
20	R	29	HIS
20	R	44	GLN
20	R	64	ASN
20	R	71	GLN
21	S	80	HIS
21	S	119	ASN
22	T	3	HIS
22	T	17	ASN
22	T	35	ASN
22	T	49	GLN
22	T	71	ASN
23	U	56	GLN
25	W	54	GLN
26	Z	23	HIS
26	Z	43	HIS
26	Z	44	HIS
26	Z	48	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2683/2880 (93%)	701 (26%)	250 (9%)
2	Y	121/123 (98%)	41 (33%)	12 (9%)
All	All	2804/3003 (93%)	742 (26%)	262 (9%)

All (742) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	7	G
1	X	13	A
1	X	14	A
1	X	15	G
1	X	23	G
1	X	34	U
1	X	45	C
1	X	48	A
1	X	49	U
1	X	50	G
1	X	54	G
1	X	62	U
1	X	63	A
1	X	69	G
1	X	70	A
1	X	71	A
1	X	72	A
1	X	73	A
1	X	74	G
1	X	82	G
1	X	83	A
1	X	84	G
1	X	89	A
1	X	90	G
1	X	91	A
1	X	97	U
1	X	99	U
1	X	100	G
1	X	101	A
1	X	107	G
1	X	108	G
1	X	111	G
1	X	112	U
1	X	116	A
1	X	117	A
1	X	118	U
1	X	123	A
1	X	127	C
1	X	129	A
1	X	136	A
1	X	137	A

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Mol	Chain	Res	Type
1	X	138	G
1	X	143	A
1	X	147	G
1	X	154	U
1	X	157	G
1	X	158	A
1	X	173	A
1	X	174	A
1	X	176	A
1	X	177	U
1	X	181	A
1	X	182	G
1	X	191	G
1	X	192	G
1	X	193	A
1	X	199	A
1	X	203	G
1	X	205	A
1	X	206	U
1	X	207	U
1	X	209	G
1	X	219	G
1	X	225	G
1	X	227	G
1	X	228	A
1	X	229	G
1	X	238	G
1	X	239	A
1	X	241	C
1	X	242	A
1	X	243	G
1	X	245	C
1	X	246	C
1	X	248	A
1	X	310	A
1	X	312	G
1	X	319	G
1	X	321	A
1	X	322	A
1	X	323	G
1	X	332	C
1	X	333	A

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Mol	Chain	Res	Type
1	X	334	G
1	X	335	A
1	X	338	G
1	X	340	G
1	X	342	G
1	X	343	A
1	X	349	G
1	X	358	C
1	X	360	A
1	X	361	G
1	X	388	G
1	X	396	U
1	X	397	U
1	X	399	G
1	X	400	U
1	X	409	G
1	X	411	C
1	X	414	A
1	X	416	U
1	X	417	C
1	X	418	C
1	X	419	G
1	X	424	G
1	X	425	A
1	X	433	G
1	X	441	A
1	X	455	A
1	X	456	C
1	X	458	G
1	X	459	A
1	X	461	A
1	X	463	C
1	X	467	U
1	X	468	A
1	X	469	G
1	X	470	U
1	X	484	G
1	X	490	A
1	X	492	G
1	X	495	C
1	X	504	G
1	X	506	G

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Mol	Chain	Res	Type
1	X	513	A
1	X	514	G
1	X	515	A
1	X	518	A
1	X	519	C
1	X	520	C
1	X	522	G
1	X	523	A
1	X	534	U
1	X	539	A
1	X	540	G
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	555	U
1	X	557	U
1	X	558	G
1	X	559	C
1	X	560	G
1	X	572	G
1	X	580	A
1	X	581	A
1	X	582	G
1	X	583	C
1	X	584	A
1	X	595	A
1	X	596	C
1	X	597	U
1	X	601	A
1	X	602	C
1	X	613	A
1	X	614	G
1	X	623	G
1	X	625	A
1	X	627	A
1	X	631	G
1	X	632	A
1	X	633	G
1	X	636	G
1	X	645	G
1	X	648	A

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Mol	Chain	Res	Type
1	X	649	G
1	X	652	C
1	X	654	A
1	X	655	A
1	X	657	A
1	X	658	G
1	X	664	C
1	X	665	A
1	X	667	U
1	X	668	A
1	X	677	G
1	X	681	A
1	X	683	A
1	X	684	C
1	X	690	A
1	X	695	G
1	X	697	G
1	X	699	G
1	X	700	C
1	X	703	A
1	X	717	G
1	X	723	C
1	X	725	C
1	X	727	U
1	X	728	G
1	X	729	A
1	X	730	C
1	X	731	A
1	X	732	G
1	X	739	G
1	X	742	G
1	X	743	A
1	X	751	G
1	X	753	U
1	X	754	G
1	X	760	U
1	X	777	A
1	X	778	G
1	X	788	G
1	X	789	G
1	X	790	A
1	X	795	A

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Mol	Chain	Res	Type
1	X	797	A
1	X	798	G
1	X	801	A
1	X	802	A
1	X	803	C
1	X	804	C
1	X	805	G
1	X	806	A
1	X	807	A
1	X	814	G
1	X	815	A
1	X	816	U
1	X	818	G
1	X	824	U
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	842	A
1	X	843	G
1	X	859	U
1	X	860	U
1	X	872	G
1	X	879	A
1	X	883	A
1	X	886	A
1	X	891	A
1	X	919	U
1	X	922	A
1	X	926	C
1	X	931	G
1	X	938	G
1	X	939	C
1	X	940	G
1	X	941	U
1	X	943	U
1	X	944	A
1	X	952	A
1	X	956	A
1	X	957	G
1	X	967	G
1	X	968	C

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Mol	Chain	Res	Type
1	X	969	U
1	X	970	A
1	X	972	C
1	X	979	A
1	X	984	A
1	X	985	G
1	X	994	A
1	X	995	A
1	X	996	C
1	X	998	C
1	X	1001	A
1	X	1002	C
1	X	1006	C
1	X	1007	A
1	X	1010	U
1	X	1014	G
1	X	1016	C
1	X	1019	U
1	X	1020	A
1	X	1022	A
1	X	1023	U
1	X	1024	G
1	X	1028	G
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1037	U
1	X	1044	U
1	X	1053	G
1	X	1054	C
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1058	G
1	X	1068	A
1	X	1069	G
1	X	1072	U
1	X	1073	G
1	X	1077	U
1	X	1081	A
1	X	1082	G
1	X	1086	C

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Mol	Chain	Res	Type
1	X	1087	C
1	X	1090	C
1	X	1094	C
1	X	1097	A
1	X	1098	G
1	X	1099	A
1	X	1100	G
1	X	1101	U
1	X	1108	U
1	X	1121	G
1	X	1122	A
1	X	1123	G
1	X	1125	G
1	X	1127	C
1	X	1128	G
1	X	1129	A
1	X	1130	U
1	X	1141	U
1	X	1143	A
1	X	1145	C
1	X	1146	G
1	X	1152	C
1	X	1153	A
1	X	1161	U
1	X	1168	G
1	X	1182	U
1	X	1184	G
1	X	1185	C
1	X	1186	G
1	X	1187	A
1	X	1189	G
1	X	1192	A
1	X	1194	U
1	X	1209	G
1	X	1223	G
1	X	1224	A
1	X	1233	A
1	X	1250	A
1	X	1251	G
1	X	1261	G
1	X	1262	U
1	X	1263	G

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Mol	Chain	Res	Type
1	X	1264	C
1	X	1266	G
1	X	1269	G
1	X	1282	A
1	X	1284	G
1	X	1285	A
1	X	1288	A
1	X	1289	A
1	X	1302	C
1	X	1313	U
1	X	1314	A
1	X	1315	A
1	X	1319	C
1	X	1326	U
1	X	1334	A
1	X	1342	U
1	X	1345	G
1	X	1346	C
1	X	1353	A
1	X	1354	A
1	X	1357	U
1	X	1358	C
1	X	1359	G
1	X	1365	U
1	X	1372	A
1	X	1378	A
1	X	1379	A
1	X	1381	G
1	X	1392	U
1	X	1399	C
1	X	1404	C
1	X	1409	U
1	X	1410	U
1	X	1412	C
1	X	1413	U
1	X	1428	G
1	X	1429	A
1	X	1430	G
1	X	1432	G
1	X	1433	A
1	X	1434	U
1	X	1439	G

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Mol	Chain	Res	Type
1	X	1440	G
1	X	1441	A
1	X	1442	C
1	X	1443	G
1	X	1460	G
1	X	1465	G
1	X	1467	U
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1474	A
1	X	1475	U
1	X	1476	G
1	X	1489	C
1	X	1490	U
1	X	1497	C
1	X	1498	G
1	X	1505	U
1	X	1506	C
1	X	1508	G
1	X	1513	U
1	X	1514	C
1	X	1523	A
1	X	1524	C
1	X	1525	A
1	X	1528	C
1	X	1529	C
1	X	1531	C
1	X	1533	G
1	X	1545	G
1	X	1548	U
1	X	1551	U
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1562	G
1	X	1563	U
1	X	1571	G
1	X	1574	A
1	X	1575	C
1	X	1576	G
1	X	1582	A

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Mol	Chain	Res	Type
1	X	1585	A
1	X	1594	U
1	X	1600	U
1	X	1601	U
1	X	1602	G
1	X	1603	A
1	X	1608	U
1	X	1609	G
1	X	1613	G
1	X	1614	C
1	X	1624	A
1	X	1625	A
1	X	1626	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1635	G
1	X	1648	C
1	X	1651	U
1	X	1656	U
1	X	1657	A
1	X	1665	C
1	X	1668	G
1	X	1685	A
1	X	1686	A
1	X	1691	G
1	X	1695	U
1	X	1699	A
1	X	1710	U
1	X	1711	C
1	X	1713	G
1	X	1714	A
1	X	1717	A
1	X	1732	U
1	X	1733	U
1	X	1734	C
1	X	1746	A
1	X	1749	G
1	X	1754	G
1	X	1755	G
1	X	1764	A
1	X	1773	C

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Mol	Chain	Res	Type
1	X	1776	A
1	X	1777	A
1	X	1782	A
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1799	A
1	X	1800	A
1	X	1801	C
1	X	1807	A
1	X	1808	C
1	X	1810	U
1	X	1811	A
1	X	1812	U
1	X	1813	A
1	X	1821	A
1	X	1825	C
1	X	1830	C
1	X	1831	G
1	X	1839	A
1	X	1840	A
1	X	1852	G
1	X	1861	G
1	X	1867	A
1	X	1874	G
1	X	1883	A
1	X	1886	G
1	X	1910	A
1	X	1912	G
1	X	1913	G
1	X	1919	A
1	X	1921	A
1	X	1923	U
1	X	1924	C
1	X	1927	U
1	X	1937	G
1	X	1938	U
1	X	1939	U
1	X	1943	A
1	X	1946	U
1	X	1947	G

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Mol	Chain	Res	Type
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1964	A
1	X	1965	U
1	X	1976	U
1	X	1980	A
1	X	2003	A
1	X	2006	G
1	X	2014	A
1	X	2015	G
1	X	2018	G
1	X	2019	C
1	X	2026	C
1	X	2033	C
1	X	2035	G
1	X	2038	C
1	X	2039	G
1	X	2043	A
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2063	A
1	X	2076	G
1	X	2078	G
1	X	2079	A
1	X	2089	C
1	X	2166	G
1	X	2171	U
1	X	2181	A
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2193	C
1	X	2195	C
1	X	2196	U
1	X	2197	U
1	X	2199	C
1	X	2204	A
1	X	2205	C

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Mol	Chain	Res	Type
1	X	2214	G
1	X	2217	G
1	X	2218	G
1	X	2228	U
1	X	2229	G
1	X	2246	A
1	X	2247	A
1	X	2257	A
1	X	2262	C
1	X	2265	A
1	X	2266	A
1	X	2268	G
1	X	2283	G
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A
1	X	2289	A
1	X	2291	U
1	X	2295	C
1	X	2298	U
1	X	2299	A
1	X	2300	G
1	X	2301	A
1	X	2305	C
1	X	2306	A
1	X	2313	G
1	X	2315	A
1	X	2323	U
1	X	2324	G
1	X	2326	C
1	X	2329	C
1	X	2330	G
1	X	2333	A
1	X	2340	C
1	X	2351	G
1	X	2358	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2374	C

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Mol	Chain	Res	Type
1	X	2381	A
1	X	2385	U
1	X	2389	G
1	X	2396	C
1	X	2397	A
1	X	2402	U
1	X	2404	A
1	X	2405	A
1	X	2406	C
1	X	2407	G
1	X	2408	G
1	X	2409	A
1	X	2410	U
1	X	2415	G
1	X	2420	C
1	X	2426	G
1	X	2427	A
1	X	2438	A
1	X	2447	G
1	X	2448	A
1	X	2453	C
1	X	2455	A
1	X	2457	A
1	X	2459	C
1	X	2461	G
1	X	2463	G
1	X	2466	G
1	X	2470	U
1	X	2477	C
1	X	2480	C
1	X	2481	G
1	X	2483	U
1	X	2484	G
1	X	2485	U
1	X	2498	U
1	X	2499	C
1	X	2508	G
1	X	2514	G
1	X	2545	A
1	X	2546	G
1	X	2548	G
1	X	2552	C

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Mol	Chain	Res	Type
1	X	2557	G
1	X	2561	G
1	X	2564	U
1	X	2565	C
1	X	2580	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2590	U
1	X	2591	C
1	X	2593	A
1	X	2594	U
1	X	2608	A
1	X	2609	G
1	X	2611	A
1	X	2613	A
1	X	2615	U
1	X	2616	U
1	X	2618	A
1	X	2621	G
1	X	2633	A
1	X	2634	G
1	X	2640	G
1	X	2642	G
1	X	2650	G
1	X	2668	U
1	X	2692	A
1	X	2693	U
1	X	2694	G
1	X	2706	U
1	X	2713	A
1	X	2718	A
1	X	2719	U
1	X	2728	A
1	X	2731	G
1	X	2732	C
1	X	2735	C
1	X	2737	A
1	X	2745	A
1	X	2758	A
1	X	2759	U
1	X	2760	G

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Mol	Chain	Res	Type
1	X	2769	C
1	X	2770	A
1	X	2771	C
1	X	2774	U
1	X	2776	U
1	X	2778	U
1	X	2779	C
1	X	2780	A
1	X	2793	G
1	X	2795	A
1	X	2796	A
1	X	2798	A
1	X	2800	C
1	X	2808	U
1	X	2824	C
1	X	2825	A
1	X	2841	U
1	X	2843	A
1	X	2846	G
1	X	2847	G
1	X	2848	A
1	X	2849	C
1	X	2854	G
1	X	2855	C
1	X	2861	A
1	X	2864	C
1	X	2866	A
1	X	2868	G
1	X	2877	A
2	Y	11	G
2	Y	14	C
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	26	G
2	Y	27	A
2	Y	28	A
2	Y	37	C
2	Y	38	C
2	Y	39	C
2	Y	42	U
2	Y	43	G

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Mol	Chain	Res	Type
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	49	C
2	Y	52	G
2	Y	53	G
2	Y	54	U
2	Y	58	G
2	Y	59	A
2	Y	69	G
2	Y	75	A
2	Y	76	U
2	Y	77	G
2	Y	86	A
2	Y	88	C
2	Y	89	G
2	Y	90	C
2	Y	91	A
2	Y	92	G
2	Y	99	G
2	Y	102	A
2	Y	106	U
2	Y	110	U
2	Y	111	C
2	Y	112	A
2	Y	115	G
2	Y	116	C
2	Y	123	U

All (262) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	13	A
1	X	33	C
1	X	34	U
1	X	48	A
1	X	61	U
1	X	62	U
1	X	70	A
1	X	71	A
1	X	73	A
1	X	74	G

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Mol	Chain	Res	Type
1	X	82	G
1	X	83	A
1	X	89	A
1	X	98	U
1	X	99	U
1	X	100	G
1	X	117	A
1	X	173	A
1	X	176	A
1	X	181	A
1	X	190	A
1	X	198	A
1	X	204	A
1	X	242	A
1	X	247	A
1	X	312	G
1	X	321	A
1	X	322	A
1	X	332	C
1	X	333	A
1	X	334	G
1	X	339	U
1	X	341	A
1	X	342	G
1	X	343	A
1	X	387	A
1	X	396	U
1	X	399	G
1	X	400	U
1	X	408	U
1	X	416	U
1	X	417	C
1	X	425	A
1	X	447	U
1	X	454	G
1	X	458	G
1	X	466	A
1	X	467	U
1	X	469	G
1	X	513	A
1	X	522	G
1	X	539	A

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Mol	Chain	Res	Type
1	X	540	G
1	X	557	U
1	X	558	G
1	X	559	C
1	X	580	A
1	X	582	G
1	X	583	C
1	X	596	C
1	X	631	G
1	X	648	A
1	X	657	A
1	X	664	C
1	X	672	C
1	X	682	G
1	X	683	A
1	X	687	G
1	X	698	A
1	X	717	G
1	X	731	A
1	X	765	C
1	X	775	U
1	X	777	A
1	X	788	G
1	X	802	A
1	X	803	C
1	X	806	A
1	X	813	A
1	X	824	U
1	X	840	U
1	X	841	G
1	X	842	A
1	X	858	G
1	X	859	U
1	X	878	C
1	X	883	A
1	X	886	A
1	X	925	U
1	X	938	G
1	X	939	C
1	X	943	U
1	X	956	A
1	X	969	U

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Mol	Chain	Res	Type
1	X	970	A
1	X	972	C
1	X	995	A
1	X	1000	G
1	X	1019	U
1	X	1036	G
1	X	1037	U
1	X	1053	G
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1072	U
1	X	1080	A
1	X	1081	A
1	X	1086	C
1	X	1096	A
1	X	1099	A
1	X	1122	A
1	X	1129	A
1	X	1139	A
1	X	1142	G
1	X	1143	A
1	X	1152	C
1	X	1185	C
1	X	1186	G
1	X	1191	G
1	X	1223	G
1	X	1249	G
1	X	1250	A
1	X	1266	G
1	X	1278	A
1	X	1288	A
1	X	1313	U
1	X	1314	A
1	X	1325	U
1	X	1333	G
1	X	1337	G
1	X	1345	G
1	X	1353	A
1	X	1357	U
1	X	1404	C
1	X	1409	U

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Mol	Chain	Res	Type
1	X	1412	C
1	X	1433	A
1	X	1434	U
1	X	1439	G
1	X	1441	A
1	X	1442	C
1	X	1459	U
1	X	1467	U
1	X	1473	U
1	X	1474	A
1	X	1475	U
1	X	1489	C
1	X	1496	G
1	X	1508	G
1	X	1513	U
1	X	1562	G
1	X	1570	C
1	X	1574	A
1	X	1575	C
1	X	1583	A
1	X	1600	U
1	X	1601	U
1	X	1602	G
1	X	1607	A
1	X	1613	G
1	X	1618	U
1	X	1624	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1685	A
1	X	1686	A
1	X	1710	U
1	X	1711	C
1	X	1732	U
1	X	1749	G
1	X	1775	A
1	X	1777	A
1	X	1790	G
1	X	1791	C
1	X	1795	C
1	X	1799	A

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Mol	Chain	Res	Type
1	X	1800	A
1	X	1810	U
1	X	1811	A
1	X	1820	G
1	X	1830	C
1	X	1839	A
1	X	1883	A
1	X	1909	U
1	X	1920	A
1	X	1921	A
1	X	1923	U
1	X	1937	G
1	X	1938	U
1	X	1953	A
1	X	1975	G
1	X	2018	G
1	X	2032	G
1	X	2075	U
1	X	2165	A
1	X	2189	A
1	X	2204	A
1	X	2217	G
1	X	2228	U
1	X	2254	C
1	X	2258	G
1	X	2261	G
1	X	2295	C
1	X	2298	U
1	X	2299	A
1	X	2305	C
1	X	2312	A
1	X	2314	A
1	X	2323	U
1	X	2343	C
1	X	2363	G
1	X	2370	G
1	X	2381	A
1	X	2396	C
1	X	2401	A
1	X	2409	A
1	X	2447	G
1	X	2482	A

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Mol	Chain	Res	Type
1	X	2497	A
1	X	2508	G
1	X	2528	G
1	X	2545	A
1	X	2560	G
1	X	2561	G
1	X	2564	U
1	X	2580	C
1	X	2593	A
1	X	2608	A
1	X	2615	U
1	X	2660	C
1	X	2669	C
1	X	2691	C
1	X	2693	U
1	X	2731	G
1	X	2736	U
1	X	2758	A
1	X	2759	U
1	X	2770	A
1	X	2778	U
1	X	2795	A
1	X	2807	U
1	X	2808	U
1	X	2824	C
1	X	2832	G
1	X	2846	G
1	X	2848	A
1	X	2854	G
1	X	2867	G
2	Y	14	C
2	Y	46	G
2	Y	47	A
2	Y	49	C
2	Y	58	G
2	Y	86	A
2	Y	90	C
2	Y	92	G
2	Y	94	G
2	Y	111	C
2	Y	116	C
2	Y	117	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 35 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	1F4	X	2929	-	60,62,62	1.25	5 (8%)	84,95,95	2.68	38 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	1F4	X	2929	-	-	34/74/119/119	1/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F4	C41-N40	4.36	1.39	1.33
32	X	2929	1F4	C52-C51	3.38	1.44	1.39
32	X	2929	1F4	C22-C9	2.72	1.58	1.52
32	X	2929	1F4	O46-C44	2.20	1.24	1.21
32	X	2929	1F4	C4-N40	2.02	1.49	1.45

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F4	C51-C47-N45	-8.14	98.37	112.99
32	X	2929	1F4	C6-O10-C11	6.63	129.97	118.18
32	X	2929	1F4	C58-C49-C50	-5.51	104.57	110.66
32	X	2929	1F4	C22-C9-C7	-5.16	103.00	111.12
32	X	2929	1F4	O43-C13-C14	5.01	119.16	107.50
32	X	2929	1F4	C21-C14-C13	5.00	120.37	111.40
32	X	2929	1F4	C49-C48-C47	-4.44	101.42	105.98
32	X	2929	1F4	C9-C7-C2	-4.36	108.70	116.11
32	X	2929	1F4	C9-C8-C14	4.30	120.20	113.61
32	X	2929	1F4	O42-C41-N40	-4.26	124.25	129.22
32	X	2929	1F4	C58-C49-C57	3.85	115.94	109.51
32	X	2929	1F4	O18-C9-C8	3.78	115.63	107.85
32	X	2929	1F4	C54-N55-C56	3.74	123.32	116.85
32	X	2929	1F4	O17-C41-N40	3.73	112.94	109.73
32	X	2929	1F4	C51-C56-N55	-3.62	118.45	124.14
32	X	2929	1F4	C22-C9-C8	-3.57	104.32	109.75
32	X	2929	1F4	C2-C3-C1	3.53	125.24	119.10
32	X	2929	1F4	O46-C44-N45	-3.49	120.22	124.26
32	X	2929	1F4	C21-C14-C8	3.47	120.06	112.55
32	X	2929	1F4	C19-C2-C7	-3.15	104.01	109.81
32	X	2929	1F4	O10-C6-C23	3.13	113.37	107.40
32	X	2929	1F4	O20-C28-O29	-2.95	102.43	110.67
32	X	2929	1F4	C57-C49-C48	-2.94	105.87	111.19
32	X	2929	1F4	C28-O20-C8	-2.90	111.22	116.25
32	X	2929	1F4	C48-C47-C51	-2.84	108.23	113.67
32	X	2929	1F4	C28-O29-C30	-2.65	108.70	112.91
32	X	2929	1F4	C7-C9-C8	2.61	113.41	110.25
32	X	2929	1F4	C31-C32-C33	2.53	113.61	109.97
32	X	2929	1F4	O15-C3-C2	-2.52	116.59	121.26
32	X	2929	1F4	C24-C5-C6	2.50	116.81	112.36
32	X	2929	1F4	C16-C1-C3	2.49	112.41	108.08
32	X	2929	1F4	C13-O43-C44	2.32	120.33	117.06
32	X	2929	1F4	C7-C2-C3	-2.20	109.54	113.32
32	X	2929	1F4	C23-C6-C5	-2.16	112.26	115.23
32	X	2929	1F4	O17-C5-C4	-2.10	101.09	103.21
32	X	2929	1F4	C31-C32-N34	-2.06	109.85	115.67
32	X	2929	1F4	C24-C5-C4	2.04	119.29	116.42
32	X	2929	1F4	O10-C11-O26	2.04	127.74	123.94

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C4-C5-C6-O10
32	X	2929	1F4	C4-C5-C6-C23
32	X	2929	1F4	O17-C5-C6-O10
32	X	2929	1F4	O17-C5-C6-C23
32	X	2929	1F4	C24-C5-C6-O10
32	X	2929	1F4	C24-C5-C6-C23
32	X	2929	1F4	O20-C8-C9-C22
32	X	2929	1F4	C7-C9-O18-C39
32	X	2929	1F4	C14-C13-O43-C44
32	X	2929	1F4	C31-C32-N34-C35
32	X	2929	1F4	C31-C32-N34-C36
32	X	2929	1F4	C33-C32-N34-C35
32	X	2929	1F4	C33-C32-N34-C36
32	X	2929	1F4	C12-C13-O43-C44
32	X	2929	1F4	C25-C23-C6-O10
32	X	2929	1F4	O43-C13-C14-C8
32	X	2929	1F4	C12-C13-C14-C8
32	X	2929	1F4	C19-C2-C7-C9
32	X	2929	1F4	C13-C14-C8-C9
32	X	2929	1F4	O46-C44-O43-C13
32	X	2929	1F4	C25-C23-C6-C5
32	X	2929	1F4	C14-C8-C9-C7
32	X	2929	1F4	C14-C8-C9-O18
32	X	2929	1F4	C14-C8-C9-C22
32	X	2929	1F4	O20-C8-C9-C7
32	X	2929	1F4	O20-C8-C9-O18
32	X	2929	1F4	N45-C44-O43-C13
32	X	2929	1F4	C22-C9-O18-C39
32	X	2929	1F4	C13-C14-C8-O20
32	X	2929	1F4	C8-C9-O18-C39
32	X	2929	1F4	C3-C2-C7-C9
32	X	2929	1F4	C4-C1-C3-C2
32	X	2929	1F4	C4-C1-C3-O15
32	X	2929	1F4	C16-C1-C3-C2

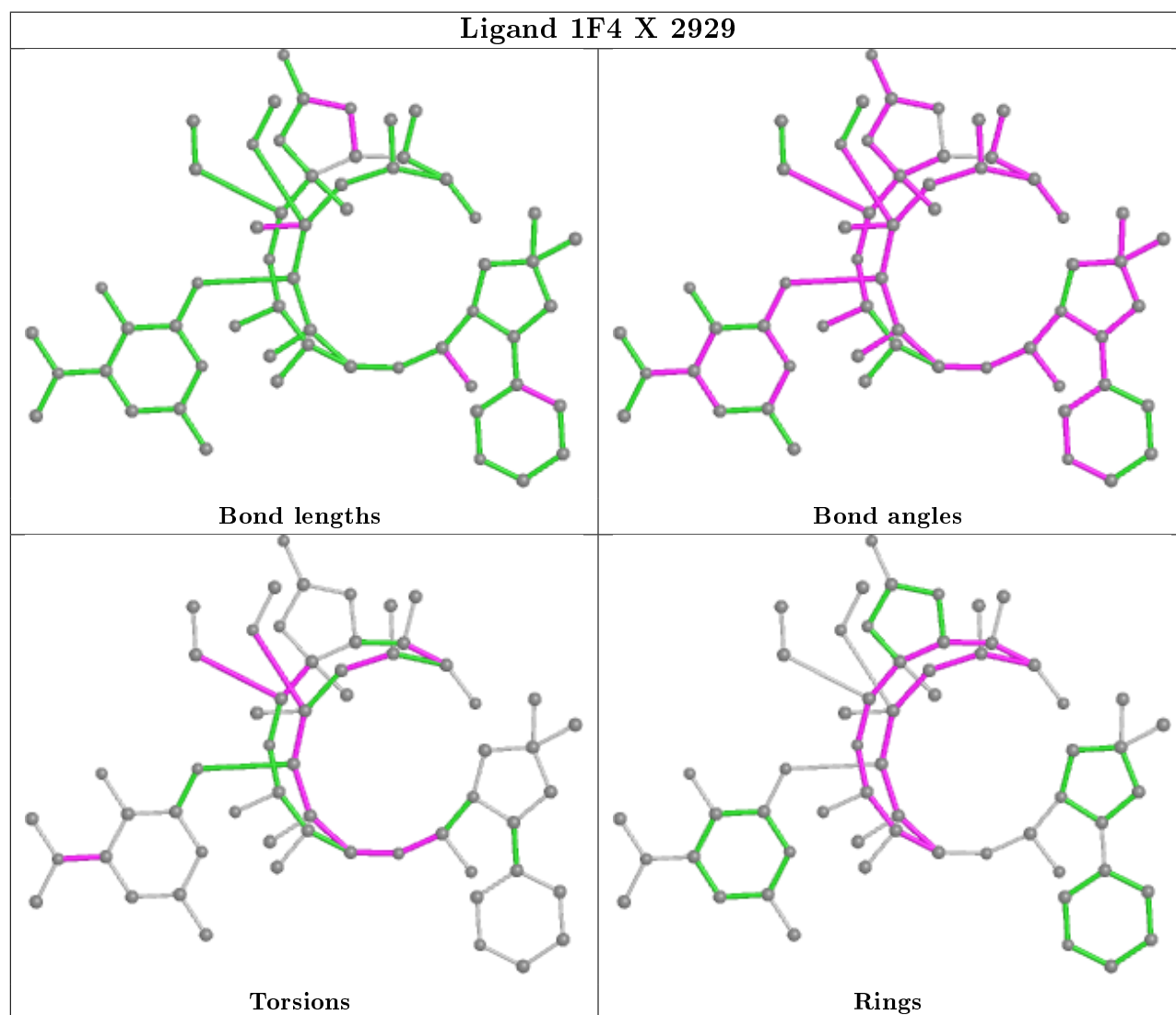
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C1-C11-C12-C13-C14-C2-C3-C4-C5-C6-C7-C8-C9-O10

1 monomer is involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2929	1F4	19	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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	X	2686/2880 (93%)	-0.14	68 (2%) 57 41	43, 92, 197, 276	0
2	Y	122/123 (99%)	-0.13	3 (2%) 57 41	83, 135, 170, 191	0
3	A	240/274 (87%)	-0.20	4 (1%) 70 55	68, 115, 146, 172	0
4	B	205/211 (97%)	-0.34	1 (0%) 91 83	45, 73, 105, 154	0
5	C	197/205 (96%)	-0.15	8 (4%) 37 24	57, 114, 154, 187	0
6	D	177/180 (98%)	-0.18	9 (5%) 28 17	146, 183, 216, 227	0
7	E	171/185 (92%)	-0.52	2 (1%) 79 66	92, 143, 192, 206	0
8	F	71/144 (49%)	1.53	19 (26%) 0 0	211, 236, 252, 257	0
9	G	142/174 (81%)	-0.32	1 (0%) 87 78	72, 97, 144, 161	0
10	H	134/134 (100%)	-0.40	0 100 100	50, 70, 97, 121	0
11	I	141/156 (90%)	0.30	11 (7%) 13 8	67, 129, 174, 204	0
12	J	136/141 (96%)	0.24	7 (5%) 28 17	74, 103, 149, 184	0
13	K	113/116 (97%)	-0.38	0 100 100	35, 60, 79, 91	0
14	L	104/114 (91%)	-0.15	1 (0%) 82 70	98, 134, 156, 168	0
15	M	108/166 (65%)	-0.62	0 100 100	50, 73, 111, 145	0
16	N	117/118 (99%)	-0.43	0 100 100	59, 90, 128, 159	0
17	O	94/100 (94%)	-0.30	2 (2%) 63 48	66, 115, 157, 173	0
18	P	127/134 (94%)	-0.50	0 100 100	50, 68, 107, 158	0
19	Q	93/95 (97%)	-0.25	2 (2%) 62 45	73, 106, 162, 195	0
20	R	110/115 (95%)	-0.16	5 (4%) 33 21	88, 117, 170, 178	0
21	S	175/237 (73%)	0.35	14 (8%) 12 7	121, 155, 175, 190	0
22	T	84/91 (92%)	0.47	10 (11%) 4 3	79, 107, 186, 200	0
23	U	72/81 (88%)	0.06	6 (8%) 11 7	92, 128, 153, 161	0
24	V	66/67 (98%)	0.02	5 (7%) 13 8	100, 132, 211, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	-0.48	1 (1%) 68 53	80, 98, 126, 152	0
26	Z	58/60 (96%)	-0.16	3 (5%) 27 17	49, 70, 105, 114	0
27	1	53/55 (96%)	2.48	19 (35%) 0 0	8, 32, 62, 93	0
28	2	46/47 (97%)	5.92	44 (95%) 0 0	3, 15, 38, 59	0
29	3	63/66 (95%)	3.45	44 (69%) 0 0	3, 25, 40, 61	0
30	4	37/37 (100%)	4.01	24 (64%) 0 0	228, 254, 266, 269	0
All	All	5997/6561 (91%)	-0.01	313 (5%) 27 17	3, 100, 196, 276	0

All (313) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	18.8
28	2	27	GLY	13.9
22	T	9	SER	13.0
30	4	25	VAL	12.8
28	2	8	ASN	12.4
29	3	35	GLY	12.4
28	2	4	THR	11.8
28	2	37	LYS	11.6
27	1	25	THR	10.8
1	X	731	A	10.5
24	V	1	MET	10.4
30	4	24	LEU	10.3
28	2	33	ARG	10.2
29	3	42	ARG	10.2
28	2	32	ALA	10.1
27	1	24	THR	9.9
28	2	24	THR	9.9
27	1	43	VAL	9.4
28	2	9	ASN	9.3
30	4	17	VAL	9.2
27	1	44	ALA	9.0
28	2	25	LYS	8.9
28	2	26	SER	8.8
30	4	29	ASN	8.6
27	1	26	LYS	8.5
28	2	29	ASN	8.4
28	2	22	MET	8.4
11	I	9	THR	8.4
1	X	1089	C	8.2

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Mol	Chain	Res	Type	RSRZ
28	2	7	PRO	8.1
28	2	2	LYS	8.0
29	3	8	LYS	7.9
29	3	32	GLN	7.8
28	2	23	LYS	7.8
27	1	23	THR	7.8
28	2	36	ALA	7.7
29	3	31	HIS	7.7
29	3	2	PRO	7.4
30	4	28	SER	7.4
29	3	22	VAL	7.3
29	3	6	THR	7.3
1	X	1091	C	7.3
28	2	11	LYS	7.2
22	T	10	SER	7.1
1	X	1090	C	7.0
28	2	6	GLN	6.7
8	F	114	ASP	6.7
30	4	34	GLN	6.6
12	J	84	MET	6.6
28	2	13	ALA	6.5
11	I	8	PRO	6.4
29	3	10	ALA	6.4
28	2	38	GLY	6.3
2	Y	123	U	6.3
3	A	203	ASN	6.2
1	X	1067	G	6.2
28	2	15	THR	6.1
30	4	6	SER	6.0
1	X	1079	G	5.9
26	Z	2	ALA	5.9
28	2	16	HIS	5.8
30	4	16	VAL	5.7
29	3	7	HIS	5.7
1	X	1106	A	5.6
30	4	35	ARG	5.6
12	J	82	THR	5.6
1	X	1086	C	5.6
28	2	28	ARG	5.6
22	T	8	GLY	5.5
8	F	137	THR	5.5
30	4	22	ARG	5.5

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Mol	Chain	Res	Type	RSRZ
30	4	23	VAL	5.4
28	2	20	ALA	5.3
1	X	248	A	5.3
29	3	27	SER	5.3
29	3	51	ALA	5.2
30	4	19	ARG	5.2
30	4	32	HIS	5.1
29	3	63	PRO	5.0
1	X	1078	A	5.0
29	3	40	GLU	4.9
11	I	4	HIS	4.9
4	B	205	SER	4.9
29	3	36	LYS	4.9
1	X	1068	A	4.9
30	4	21	GLY	4.9
28	2	5	TYR	4.9
11	I	10	PRO	4.8
30	4	20	HIS	4.8
8	F	125	ASN	4.7
27	1	41	ASP	4.7
11	I	52	GLY	4.7
11	I	5	ASP	4.6
28	2	41	GLN	4.6
24	V	3	PRO	4.6
19	Q	64	ARG	4.5
1	X	1107	A	4.5
11	I	29	THR	4.5
8	F	98	LYS	4.5
21	S	29	ASN	4.5
1	X	2776	U	4.5
29	3	34	THR	4.5
24	V	4	SER	4.4
1	X	1084	A	4.4
30	4	36	GLN	4.4
5	C	47	THR	4.4
30	4	27	CYS	4.3
29	3	9	MET	4.3
12	J	85	GLY	4.3
5	C	44	SER	4.2
29	3	33	ASN	4.2
3	A	250	TRP	4.2
20	R	100	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
28	2	40	HIS	4.2
1	X	1077	U	4.1
1	X	730	C	4.1
8	F	108	ALA	4.1
29	3	3	LYS	4.1
1	X	2289	A	4.0
29	3	59	LYS	4.0
29	3	60	LEU	4.0
29	3	18	GLY	4.0
28	2	43	THR	3.9
29	3	5	LYS	3.9
1	X	1099	A	3.9
29	3	39	ASP	3.9
22	T	6	GLY	3.8
8	F	111	LYS	3.8
1	X	1186	G	3.8
6	D	42	SER	3.8
6	D	43	SER	3.8
28	2	3	ARG	3.8
8	F	113	PRO	3.8
1	X	1073	G	3.7
21	S	28	ASN	3.7
5	C	123	PHE	3.7
29	3	64	ARG	3.7
28	2	34	ARG	3.7
11	I	6	LEU	3.7
27	1	47	HIS	3.6
1	X	1085	G	3.6
8	F	84	ILE	3.6
8	F	92	ASN	3.6
1	X	1094	C	3.6
27	1	11	LYS	3.6
1	X	1104	G	3.5
29	3	4	MET	3.5
24	V	2	LYS	3.5
28	2	1	MET	3.5
28	2	10	ARG	3.5
22	T	15	ASP	3.5
21	S	23	ALA	3.4
29	3	19	THR	3.4
20	R	99	VAL	3.4
1	X	74	G	3.4

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Mol	Chain	Res	Type	RSRZ
22	T	17	ASN	3.4
28	2	19	ARG	3.4
23	U	27	ASP	3.4
1	X	1080	A	3.3
5	C	197	GLU	3.3
20	R	57	ASN	3.3
1	X	1081	A	3.3
29	3	47	GLY	3.3
23	U	47	HIS	3.3
29	3	55	TRP	3.3
30	4	26	ILE	3.3
12	J	81	GLU	3.2
1	X	2777	A	3.2
21	S	24	TYR	3.2
27	1	20	PHE	3.2
30	4	18	ARG	3.2
30	4	7	VAL	3.2
21	S	143	ILE	3.2
8	F	107	ILE	3.2
2	Y	68	A	3.1
28	2	12	ARG	3.1
23	U	16	ASN	3.1
1	X	891	A	3.1
22	T	4	LYS	3.1
1	X	1114	A	3.1
27	1	22	TYR	3.1
30	4	10	MET	3.1
28	2	30	ILE	3.1
28	2	17	GLY	3.1
28	2	45	SER	3.0
27	1	31	THR	3.0
1	X	728	G	3.0
8	F	112	MET	3.0
8	F	100	ASN	3.0
21	S	165	GLU	3.0
8	F	121	GLU	3.0
1	X	1098	G	3.0
29	3	53	ALA	3.0
5	C	20	PRO	3.0
5	C	198	GLU	3.0
8	F	97	GLY	2.9
27	1	14	SER	2.9

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Mol	Chain	Res	Type	RSRZ
6	D	146	VAL	2.9
1	X	2329	C	2.9
1	X	1072	U	2.9
30	4	5	SER	2.9
11	I	33	GLY	2.9
28	2	46	ASP	2.9
2	Y	2	C	2.9
29	3	57	ARG	2.9
7	E	5	GLY	2.8
1	X	1109	A	2.8
29	3	17	THR	2.8
27	1	9	ILE	2.8
1	X	358	C	2.7
29	3	26	LYS	2.7
6	D	145	MET	2.7
11	I	63	ARG	2.7
1	X	225	G	2.7
29	3	11	LYS	2.7
27	1	27	ASN	2.7
19	Q	94	GLN	2.7
1	X	1951	G	2.7
21	S	15	ASP	2.7
1	X	1088	A	2.7
1	X	1087	C	2.6
7	E	43	VAL	2.6
9	G	97	ASP	2.6
27	1	46	LYS	2.6
29	3	25	PHE	2.6
17	O	41	GLY	2.6
1	X	435	A	2.6
22	T	5	LYS	2.6
6	D	85	VAL	2.6
21	S	144	GLY	2.6
26	Z	59	ALA	2.6
3	A	261	ARG	2.6
22	T	7	VAL	2.5
1	X	169	C	2.5
1	X	170	U	2.5
1	X	1187	A	2.5
1	X	2287	G	2.5
1	X	2174	G	2.5
21	S	12	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
29	3	37	SER	2.5
8	F	85	GLY	2.5
12	J	21	ASP	2.5
21	S	124	ALA	2.5
6	D	26	MET	2.4
1	X	361	G	2.4
12	J	7	ARG	2.4
6	D	147	ASP	2.4
1	X	1093	U	2.4
1	X	727	U	2.4
8	F	110	THR	2.4
28	2	44	VAL	2.4
29	3	61	MET	2.4
21	S	31	SER	2.4
29	3	50	LEU	2.3
1	X	2775	U	2.3
28	2	31	LEU	2.3
29	3	38	GLY	2.3
28	2	21	ARG	2.3
28	2	42	LEU	2.3
1	X	2089	C	2.3
1	X	1115	C	2.3
1	X	1524	C	2.3
21	S	163	ASP	2.3
5	C	48	ARG	2.3
1	X	1103	C	2.3
1	X	2088	U	2.2
1	X	2778	U	2.2
17	O	39	PHE	2.2
23	U	25	ARG	2.2
1	X	1913	G	2.2
20	R	98	ILE	2.2
1	X	356	A	2.2
23	U	39	LYS	2.2
29	3	24	ALA	2.2
29	3	62	LEU	2.2
27	1	42	PRO	2.2
28	2	14	LYS	2.2
1	X	729	A	2.1
21	S	27	GLU	2.1
1	X	558	G	2.1
26	Z	3	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
8	F	138	VAL	2.1
14	L	97	HIS	2.1
21	S	164	PRO	2.1
25	W	6	VAL	2.1
28	2	39	ARG	2.1
1	X	665	A	2.1
29	3	48	PHE	2.1
30	4	14	CYS	2.1
23	U	28	GLY	2.1
1	X	1110	G	2.1
20	R	102	LYS	2.1
1	X	1076	U	2.1
27	1	49	VAL	2.1
1	X	2323	U	2.1
6	D	134	GLU	2.1
29	3	45	GLY	2.1
24	V	6	MET	2.1
29	3	44	LYS	2.1
3	A	91	ARG	2.1
8	F	90	THR	2.1
1	X	2270	U	2.1
5	C	19	LEU	2.1
1	X	483	A	2.0
12	J	86	LYS	2.0
1	X	2567	G	2.0
1	X	1121	G	2.0
30	4	4	ARG	2.0
1	X	887	G	2.0
6	D	144	ASP	2.0
22	T	11	LYS	2.0
8	F	126	THR	2.0
11	I	31	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

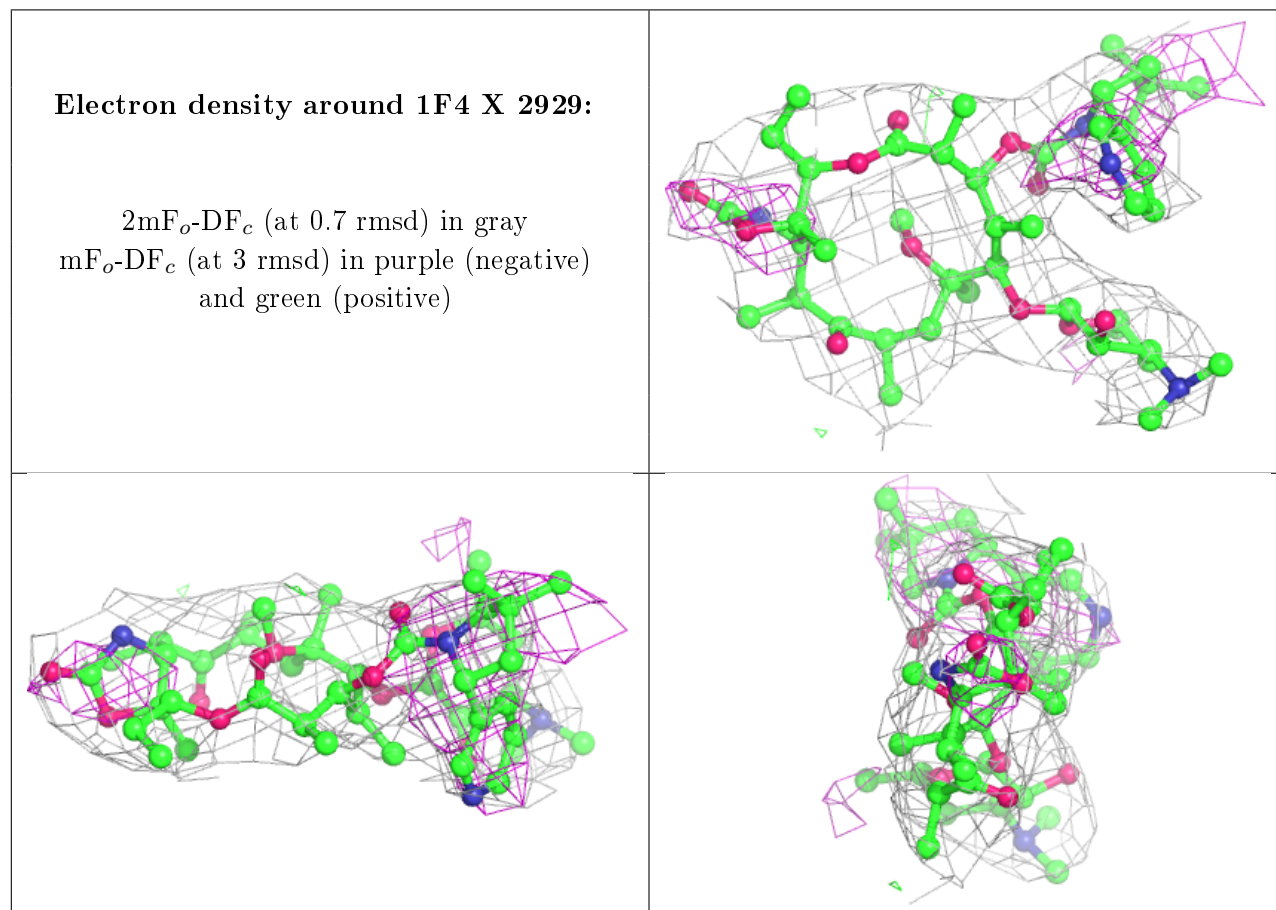
There are no carbohydrates in this entry.

6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	X	2909	1/1	0.34	0.62	97,97,97,97	0
31	MG	Y	204	1/1	0.35	0.93	86,86,86,86	0
31	MG	X	2913	1/1	0.37	1.00	60,60,60,60	0
31	MG	X	2903	1/1	0.45	0.62	89,89,89,89	0
31	MG	X	2901	1/1	0.53	0.69	50,50,50,50	0
31	MG	X	2920	1/1	0.54	0.43	113,113,113,113	0
31	MG	X	2928	1/1	0.58	0.77	61,61,61,61	0
31	MG	X	2927	1/1	0.68	0.53	64,64,64,64	0
31	MG	X	2912	1/1	0.70	0.59	71,71,71,71	0
31	MG	X	2911	1/1	0.77	0.40	68,68,68,68	0
31	MG	X	2926	1/1	0.79	1.78	45,45,45,45	0
31	MG	X	2924	1/1	0.80	1.08	70,70,70,70	0
31	MG	Y	203	1/1	0.81	0.92	59,59,59,59	0
31	MG	X	2908	1/1	0.82	2.35	37,37,37,37	0
31	MG	X	2915	1/1	0.84	0.73	57,57,57,57	0
31	MG	X	2918	1/1	0.84	1.23	42,42,42,42	0
31	MG	Y	206	1/1	0.84	0.29	78,78,78,78	0
31	MG	X	2916	1/1	0.86	1.17	37,37,37,37	0
31	MG	Y	202	1/1	0.88	1.42	88,88,88,88	0
31	MG	X	2905	1/1	0.89	0.49	65,65,65,65	0
31	MG	X	2921	1/1	0.90	0.71	80,80,80,80	0
31	MG	X	2919	1/1	0.92	0.92	30,30,30,30	0
31	MG	X	2904	1/1	0.92	0.29	110,110,110,110	0
31	MG	Y	205	1/1	0.92	0.40	82,82,82,82	0
31	MG	Y	201	1/1	0.93	0.44	98,98,98,98	0
31	MG	X	2902	1/1	0.93	0.31	94,94,94,94	0
31	MG	X	2906	1/1	0.94	0.94	58,58,58,58	0
31	MG	X	2917	1/1	0.94	1.09	55,55,55,55	0
31	MG	X	2922	1/1	0.95	0.84	44,44,44,44	0
31	MG	X	2914	1/1	0.96	0.65	27,27,27,27	0
31	MG	X	2907	1/1	0.96	0.81	51,51,51,51	0
32	1F4	X	2929	58/58	0.96	0.21	20,20,20,20	0
31	MG	X	2923	1/1	0.96	0.34	34,34,34,34	0
31	MG	X	2925	1/1	0.97	0.26	122,122,122,122	0
31	MG	M	201	1/1	0.98	1.39	23,23,23,23	0
31	MG	X	2910	1/1	0.99	0.69	41,41,41,41	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.