Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:05 pm BST

PDB ID	:	4IOA
Title	:	Crystal structure of compound 4e bound to large ribosomal subunit (50S) from Deinococcus radiodurans
Authors	:	Han, S.; Marr, E.S.
Deposited on	:	2013-01-07
Resolution	:	3.20 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:

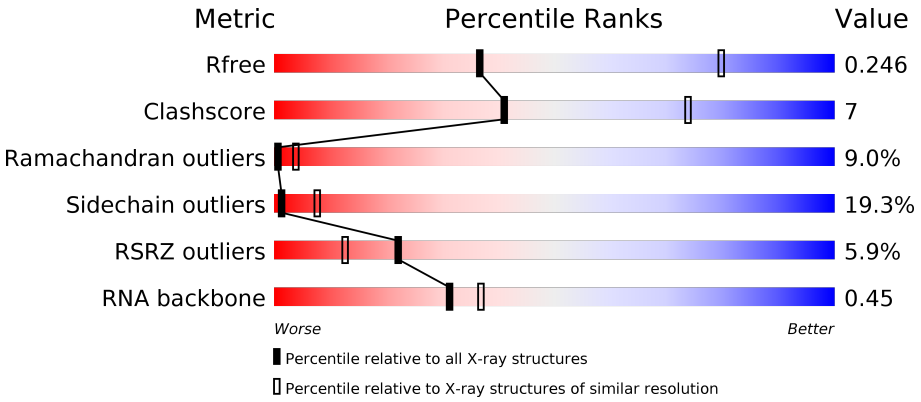
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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% 36% 34% 19% • 7%
2	Y	123	2% 40% 42% 15% • •
3	A	274	2% 48% 30% 8% • 12%
4	B	211	% 67% 21% 9% •

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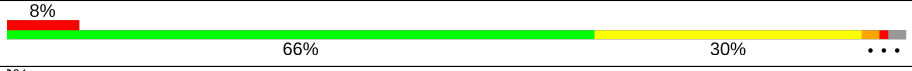
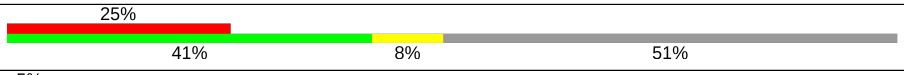
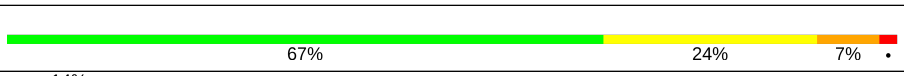
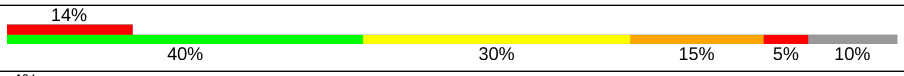
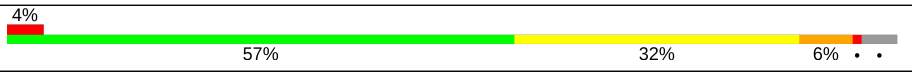
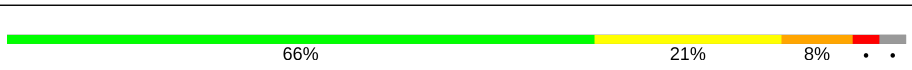
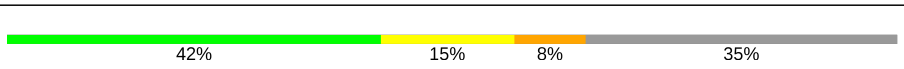
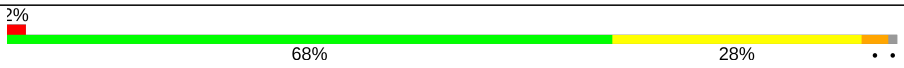
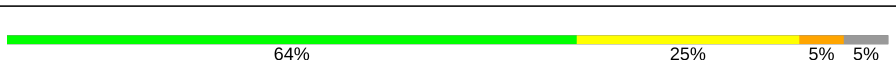
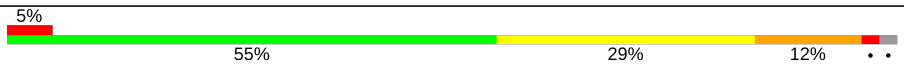
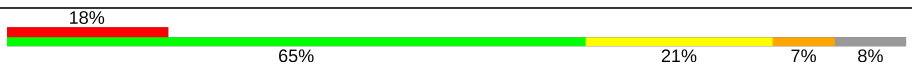
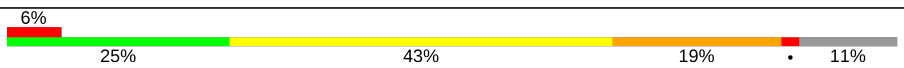
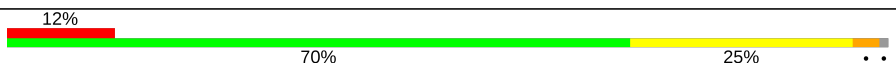
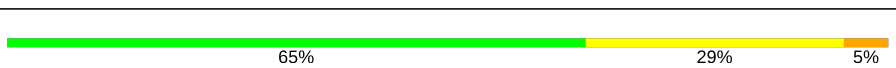
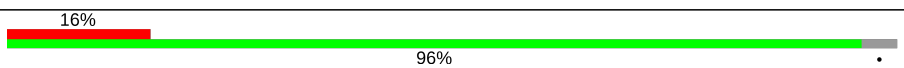
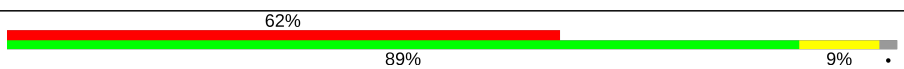
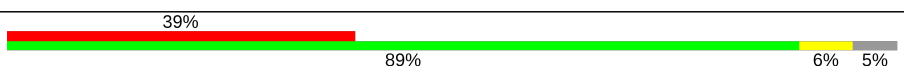
Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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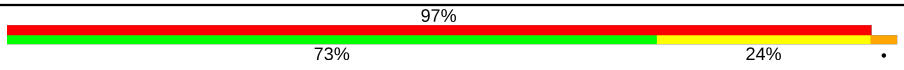
Mol	Chain	Length	Quality of chain
30	4	37	

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	2904	-	-	-	X
31	MG	X	2905	-	-	-	X
31	MG	X	2922	-	-	-	X
31	MG	Y	203	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83879 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
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

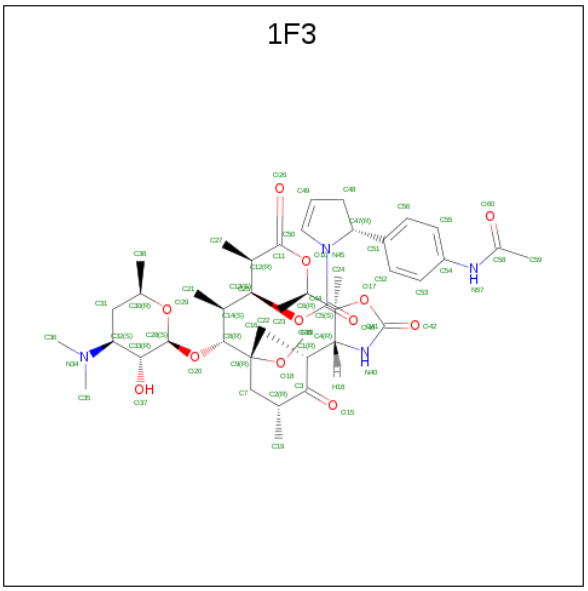
- Molecule 30 is a protein called 50S ribosomal protein L36.

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	30	Total Mg 30 30	0	0
31	Y	5	Total Mg 5 5	0	0

- Molecule 32 is (3aS,4R,7R,8S,9S,10R,11R,13R,15R,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)-2-[4-(acetylamino)phenyl]-2,3-dihydro-1H-pyrrole-1-carboxylate (three-letter code: 1F3) (formula: $C_{44}H_{66}N_4O_{12}$).



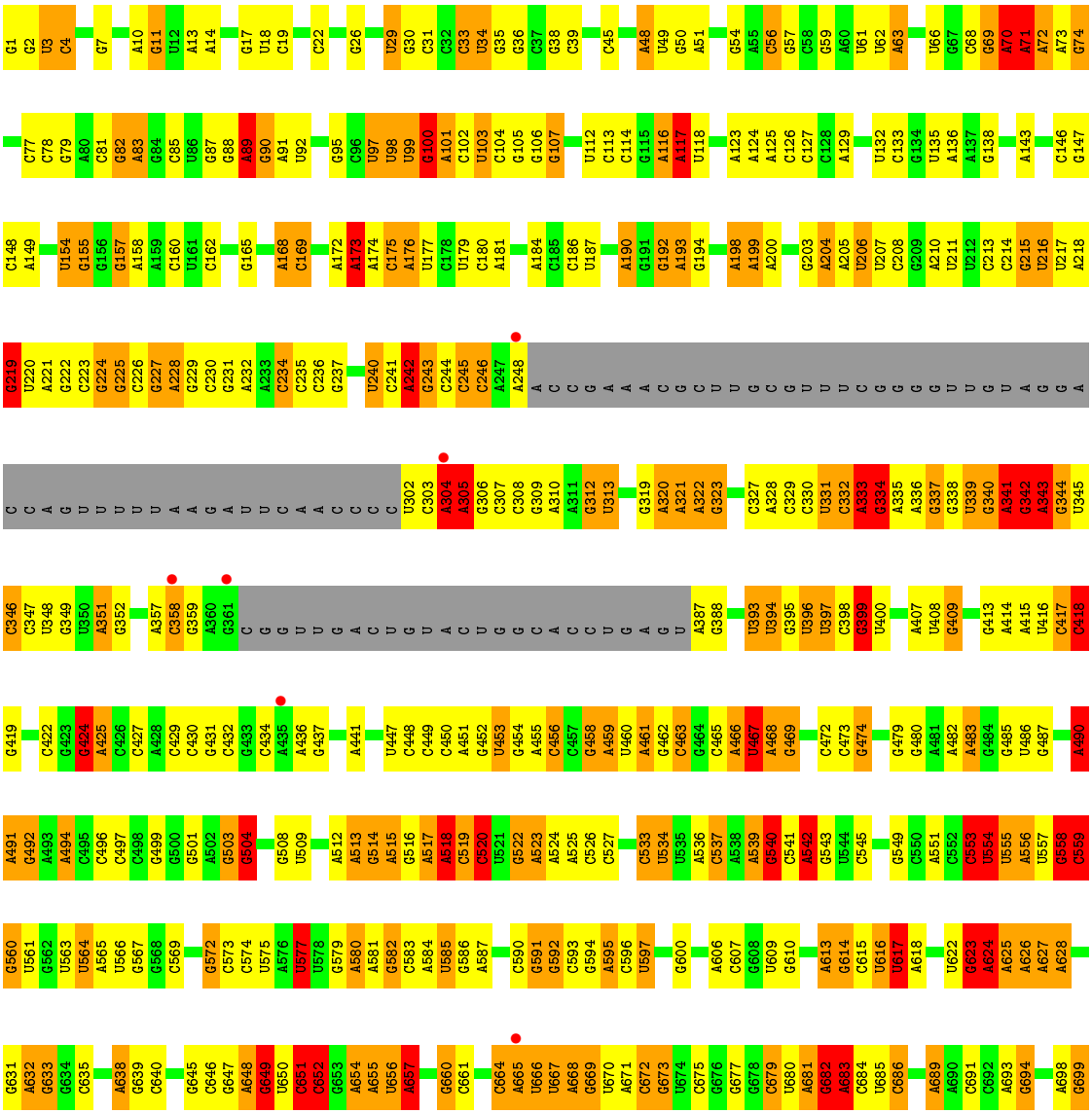
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			60	44	4	12		

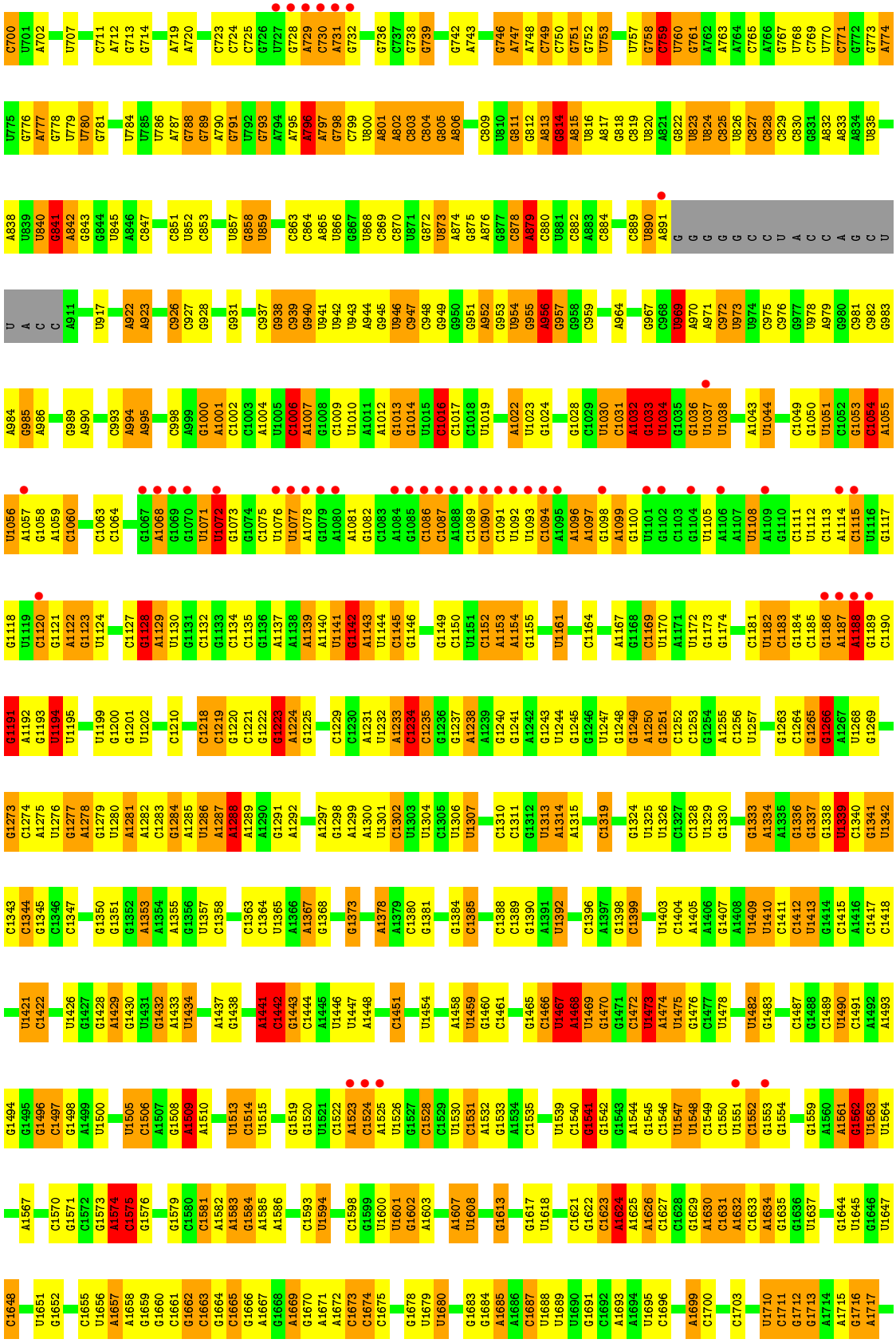
3 Residue-property plots (i)

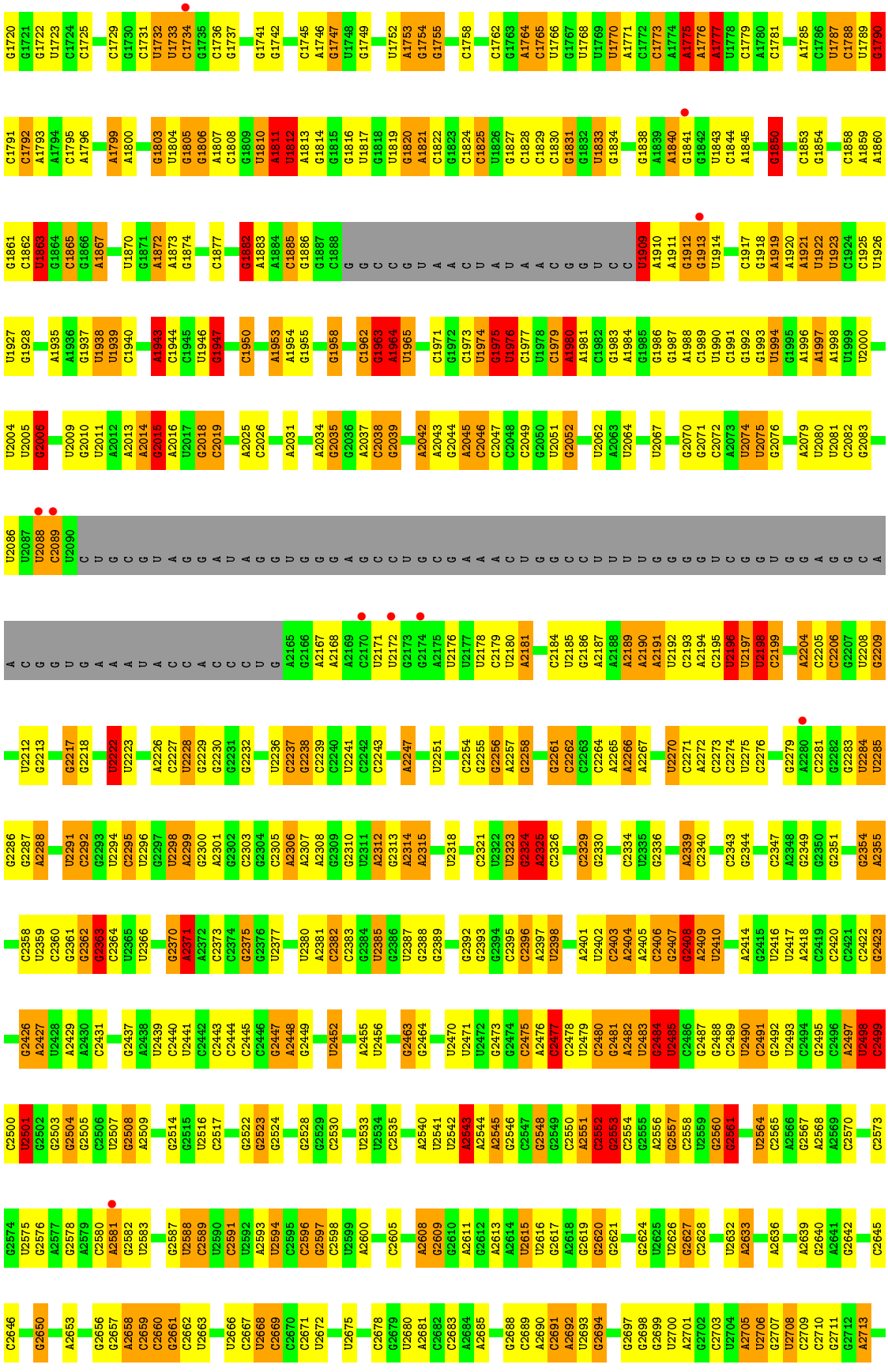
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

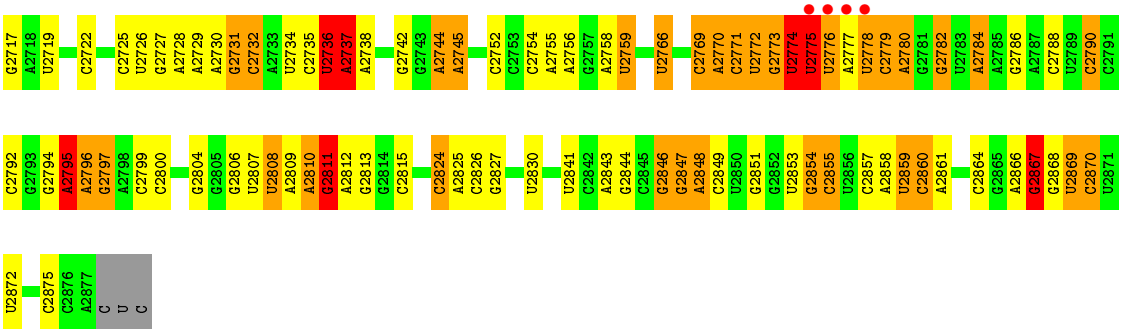
- Molecule 1: 23S ribosomal RNA

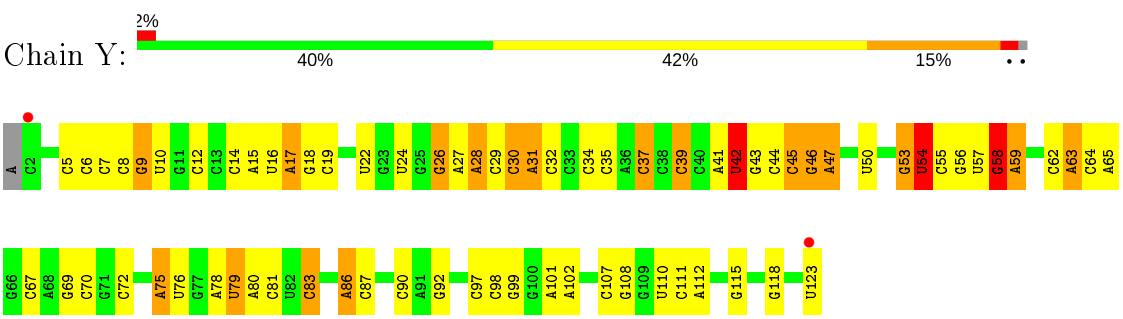
Chain X: 2% 36% 34% 19% 7%









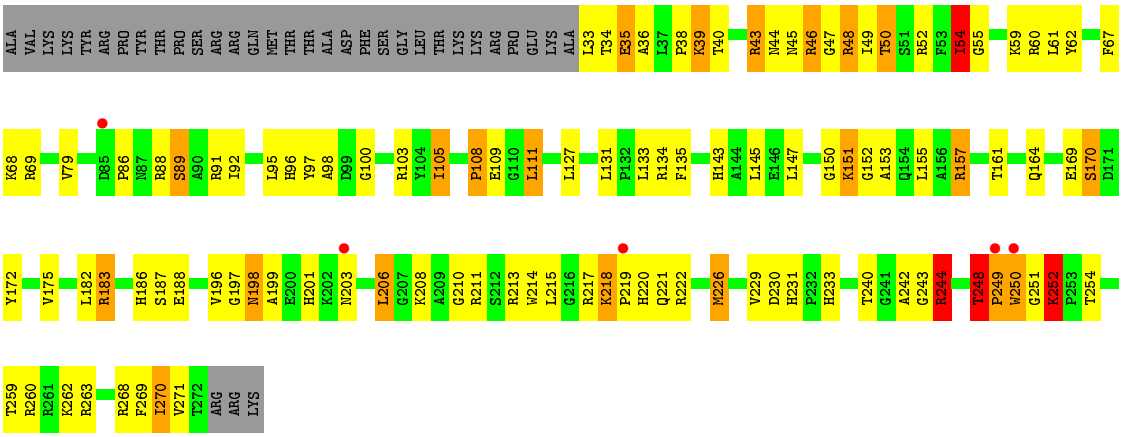


• Molecule 2: 5S ribosomal RNA

Chain Y:

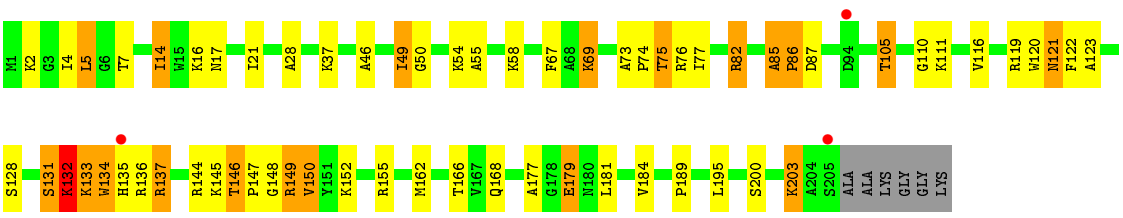
• Molecule 3: 50S ribosomal protein L2

Chain A:

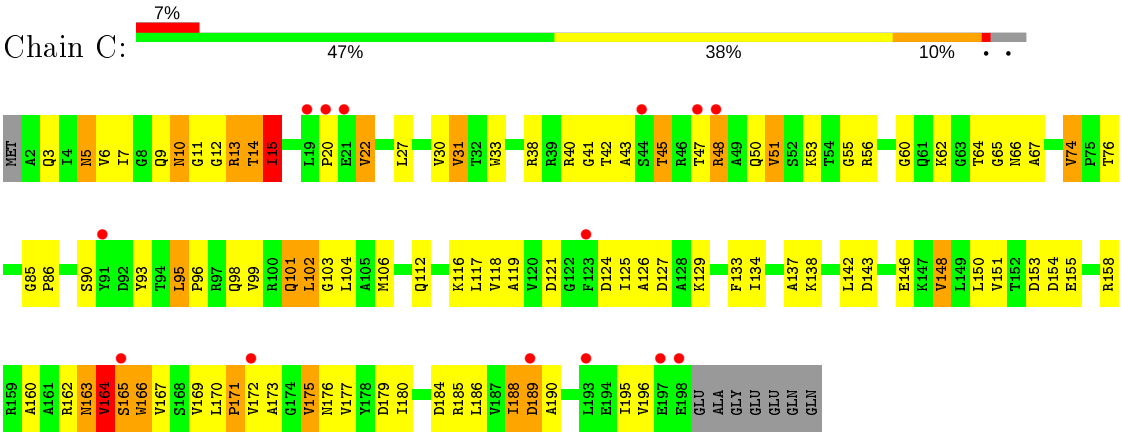


• Molecule 4: 50S ribosomal protein L3

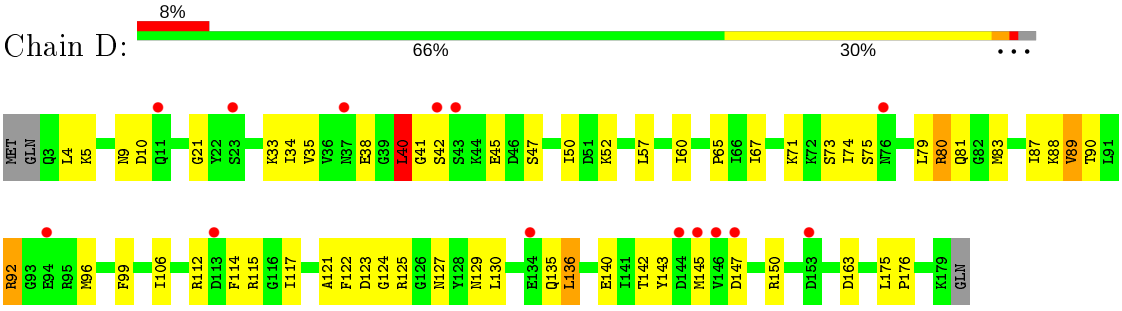
Chain B:



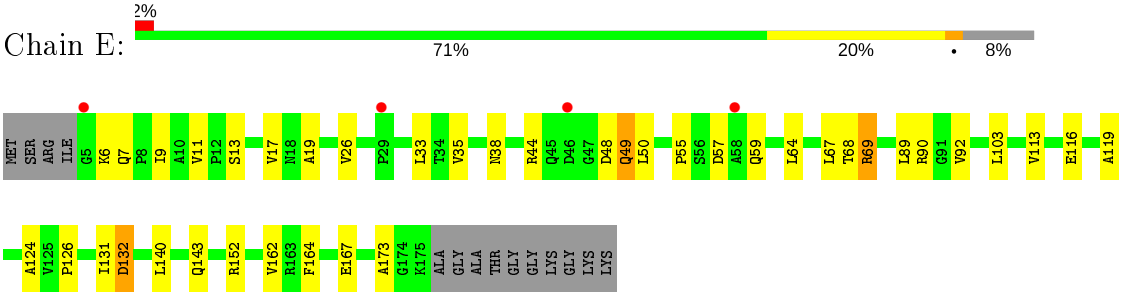
• Molecule 5: 50S ribosomal protein L4



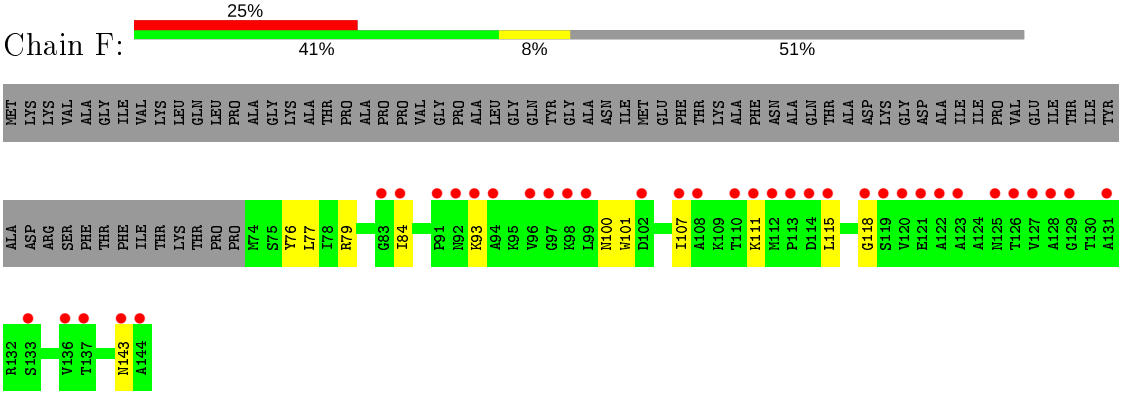
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6

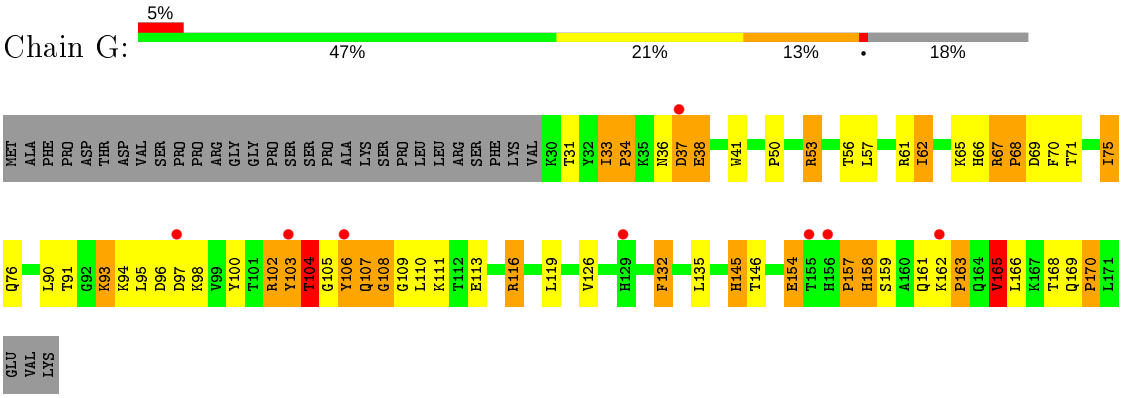


- Molecule 8: 50S ribosomal protein L11



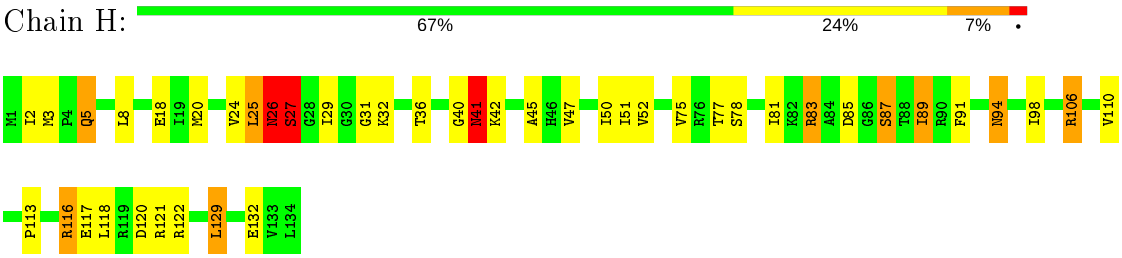
- Molecule 9: 50S ribosomal protein L13

Chain G:



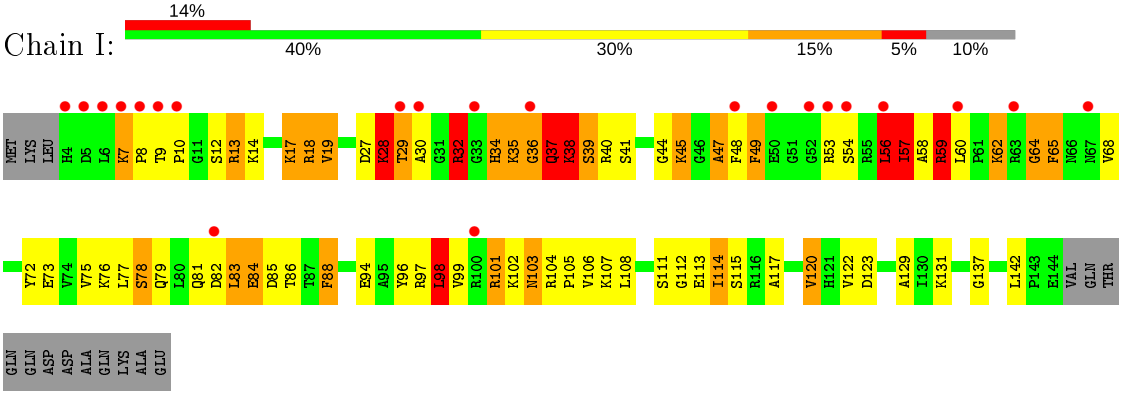
• Molecule 10: 50S ribosomal protein L14

Chain H:



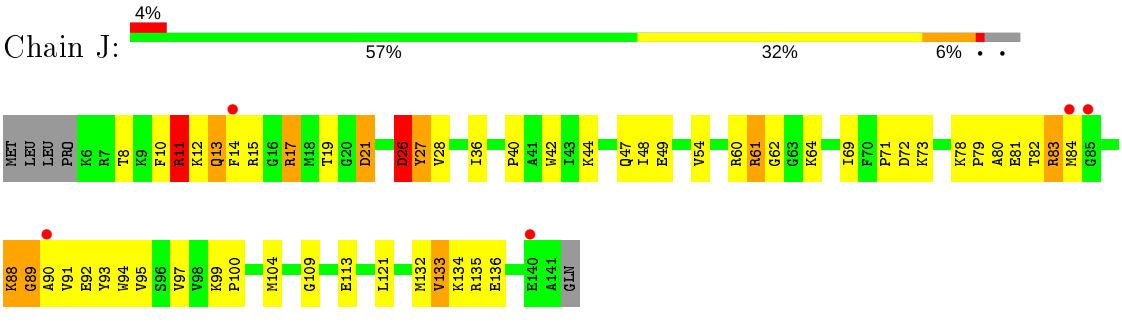
• Molecule 11: 50S ribosomal protein L15

Chain I:



• Molecule 12: 50S ribosomal protein L16

Chain J:

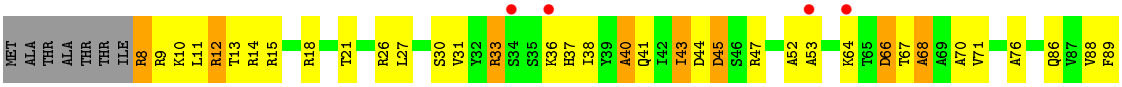


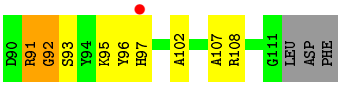
• Molecule 13: 50S ribosomal protein L17

Chain K:

- Molecule 14: 50S ribosomal protein L18

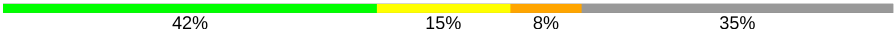
Chain L:

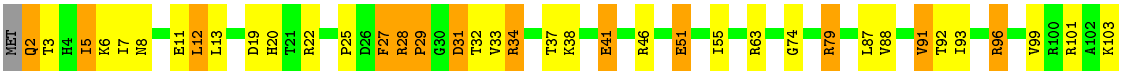




- Molecule 15: 50S ribosomal protein L19

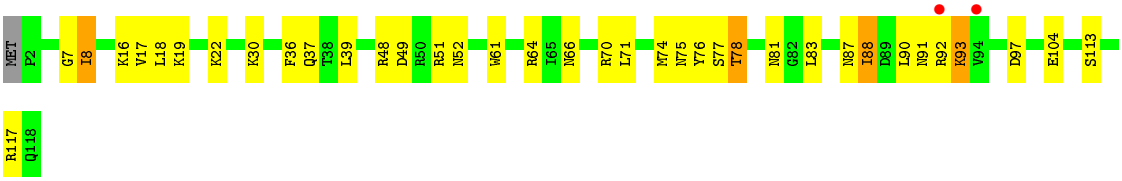
Chain M:





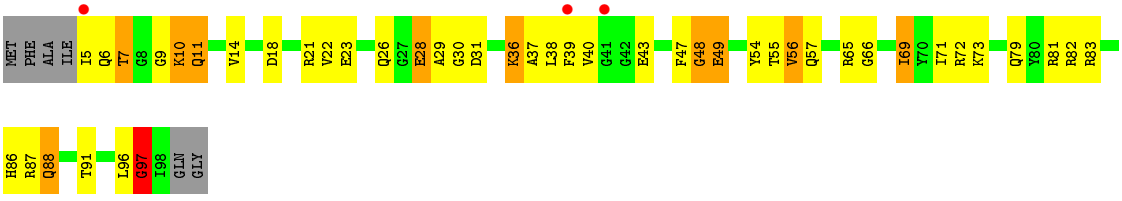
- Molecule 16: 50S ribosomal protein L20

Chain N:



- Molecule 17: 50S ribosomal protein L21

Chain O:

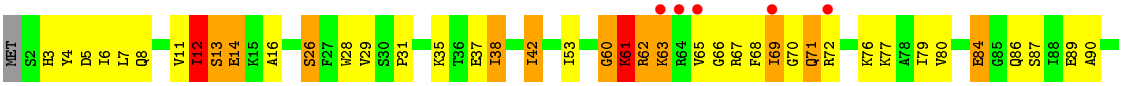


- Molecule 18: 50S ribosomal protein L22

Chain P:

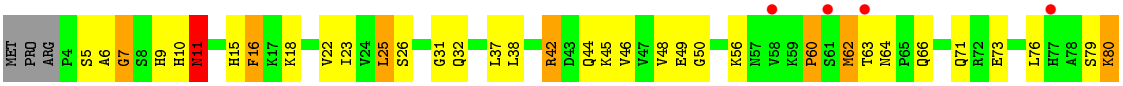
• Molecule 19: 50S ribosomal protein L23

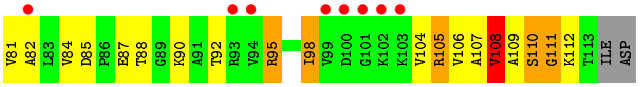
Chain Q:



• Molecule 20: 50S ribosomal protein L24

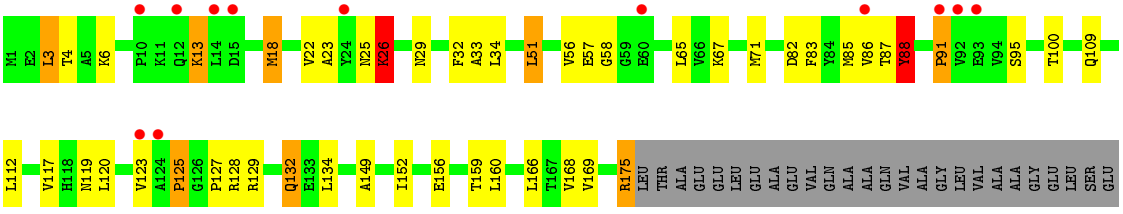
Chain R:





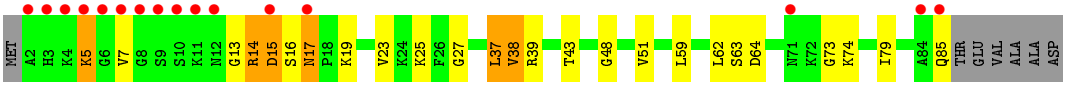
• Molecule 21: 50S ribosomal protein L25

Chain S:



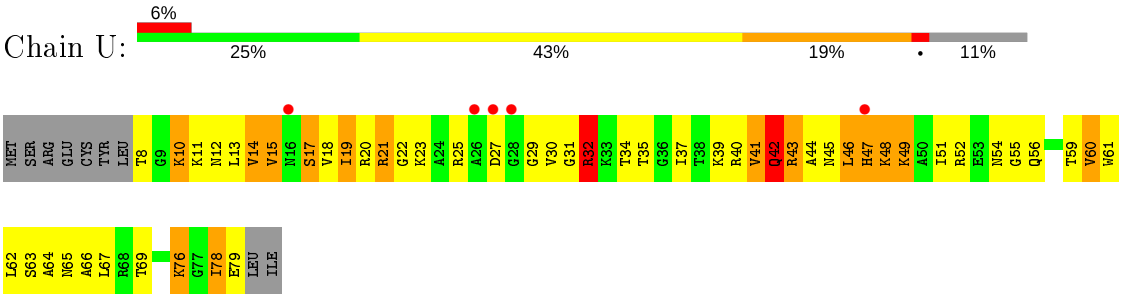
• Molecule 22: 50S ribosomal protein L27

Chain T:



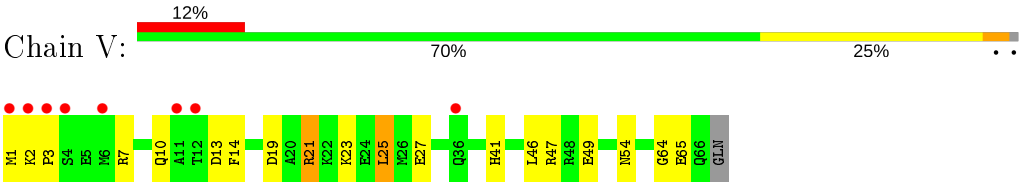
• Molecule 23: 50S ribosomal protein L28

Chain U:



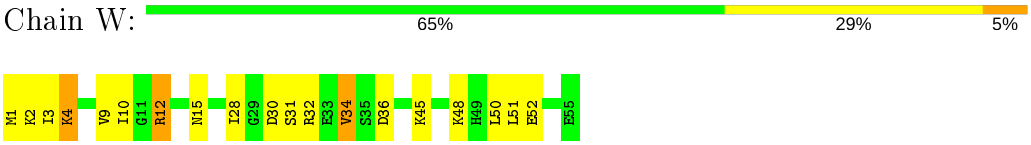
- Molecule 24: 50S ribosomal protein L29

Chain V:



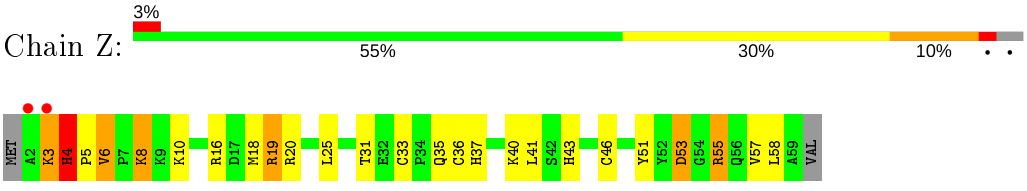
- Molecule 25: 50S ribosomal protein L30

Chain W:



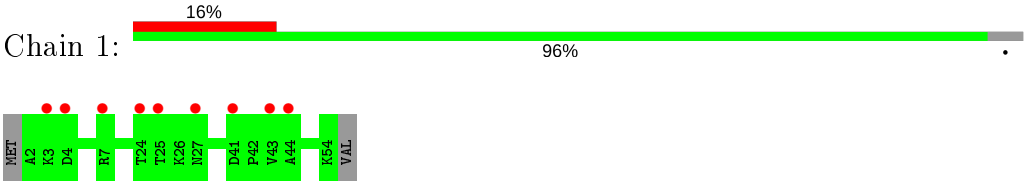
- Molecule 26: 50S ribosomal protein L32

Chain Z:



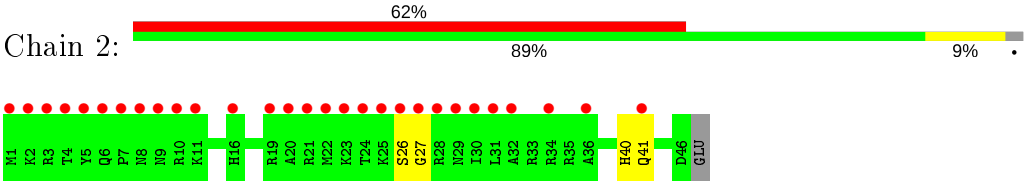
- Molecule 27: 50S ribosomal protein L33

Chain 1:



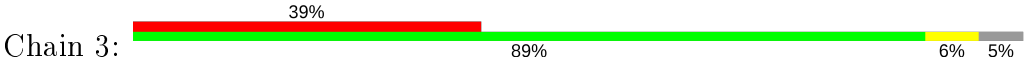
- Molecule 28: 50S ribosomal protein L34

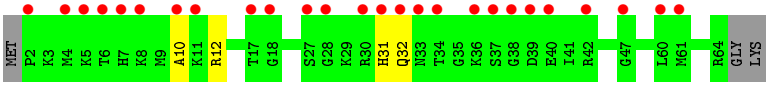
Chain 2:



- Molecule 29: 50S ribosomal protein L35

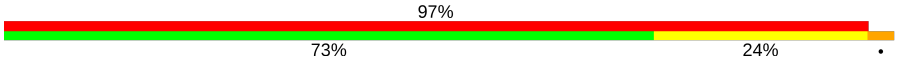
Chain 3:

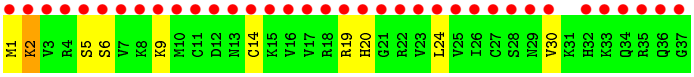




- Molecule 30: 50S ribosomal protein L36

Chain 4:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	169.77Å 406.66Å 696.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.38 – 3.23	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 89.8 (30.38-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 3.24Å)	Xtriage
Refinement program	autobuster	Depositor
R, R_{free}	0.197 , 0.230 0.211 , 0.246	Depositor DCC
R_{free} test set	17364 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	80.0	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 91.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	83879	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, 1F3

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	1.00	38/64561 (0.1%)	1.86	1965/100708 (2.0%)
2	Y	1.02	0/2904	1.68	66/4525 (1.5%)
3	A	0.62	0/1862	0.96	2/2510 (0.1%)
4	B	0.60	0/1567	0.96	2/2105 (0.1%)
5	C	0.63	0/1529	0.95	1/2070 (0.0%)
6	D	0.47	0/1419	0.67	0/1903
7	E	0.44	0/1308	0.68	0/1771
8	F	0.47	0/508	0.64	0/683
9	G	0.64	0/1138	1.01	4/1539 (0.3%)
10	H	0.55	0/1007	0.84	1/1352 (0.1%)
11	I	0.73	0/1081	1.11	8/1448 (0.6%)
12	J	0.65	0/1113	0.92	2/1486 (0.1%)
13	K	0.80	2/886 (0.2%)	0.99	3/1188 (0.3%)
14	L	0.57	0/785	0.95	1/1048 (0.1%)
15	M	0.65	1/884 (0.1%)	0.98	2/1186 (0.2%)
16	N	0.51	0/994	0.78	0/1323
17	O	0.56	0/750	0.96	1/1000 (0.1%)
18	P	0.56	0/1027	0.82	0/1373
19	Q	0.62	0/737	1.04	4/988 (0.4%)
20	R	0.64	0/835	0.99	0/1121
21	S	0.49	0/1370	0.73	0/1862
22	T	0.53	0/633	0.85	0/838
23	U	0.75	0/556	1.12	2/741 (0.3%)
24	V	0.47	0/537	0.69	0/714
25	W	0.46	0/426	0.79	0/568
26	Z	0.65	0/469	0.97	0/629
30	4	0.48	0/298	0.72	0/390
All	All	0.91	41/91184 (0.0%)	1.68	2064/137069 (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	6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	540	G	C2-N3	9.96	1.40	1.32
1	X	774	A	C5-C4	9.11	1.45	1.38
1	X	774	A	N7-C5	-7.92	1.34	1.39
1	X	2018	G	N9-C8	7.57	1.43	1.37
1	X	542	A	N7-C5	-7.47	1.34	1.39
1	X	1333	G	N9-C4	-6.86	1.32	1.38
1	X	537	C	N1-C2	6.71	1.46	1.40
1	X	774	A	N1-C2	6.70	1.40	1.34
1	X	540	G	N3-C4	6.67	1.40	1.35
1	X	1946	U	C1'-N1	6.67	1.58	1.48
1	X	774	A	N3-C4	6.56	1.38	1.34
13	K	3	HIS	CA-C	6.52	1.70	1.52
1	X	1980	A	N7-C5	-6.30	1.35	1.39
13	K	52	ILE	CG1-CD1	6.21	1.93	1.50
1	X	699	G	N9-C4	-6.18	1.33	1.38
15	M	29	PRO	CA-C	5.88	1.64	1.52
1	X	462	G	C6-O6	5.86	1.29	1.24
1	X	1468	A	N9-C4	5.79	1.41	1.37
1	X	343	A	N9-C4	5.76	1.41	1.37
1	X	796	A	N9-C4	-5.72	1.34	1.37
1	X	1467	U	C1'-N1	5.72	1.57	1.48
1	X	1288	A	C4'-C3'	-5.64	1.47	1.52
1	X	2485	U	N1-C2	5.64	1.43	1.38
1	X	434	C	C1'-N1	5.62	1.57	1.48
1	X	1688	U	C2-N3	5.54	1.41	1.37
1	X	2321	C	C1'-N1	5.41	1.56	1.48
1	X	540	G	C3'-O3'	5.38	1.49	1.42
1	X	537	C	C4-C5	5.34	1.47	1.43
1	X	868	U	C1'-N1	5.33	1.56	1.48
1	X	1223	G	C2-N3	5.30	1.36	1.32
1	X	2482	A	N3-C4	5.27	1.38	1.34
1	X	1688	U	N3-C4	5.25	1.43	1.38
1	X	327	C	C1'-N1	5.24	1.56	1.48
1	X	2485	U	C1'-N1	5.22	1.56	1.48
1	X	78	C	C1'-N1	5.21	1.56	1.48
1	X	358	C	C1'-N1	5.21	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2795	A	N3-C4	5.19	1.38	1.34
1	X	1522	C	C1'-N1	5.09	1.56	1.48
1	X	1688	U	C4-O4	5.05	1.27	1.23
1	X	559	C	C3'-O3'	5.03	1.49	1.42
1	X	2072	C	C1'-N1	5.03	1.56	1.48

All (2064) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1288	A	C1'-O4'-C4'	-38.76	78.89	109.90
1	X	1288	A	C5'-C4'-O4'	20.93	134.22	109.10
1	X	1716	G	P-O3'-C3'	19.09	142.60	119.70
1	X	1288	A	C4'-C3'-C2'	-19.04	83.56	102.60
1	X	2808	U	O4'-C1'-N1	17.91	122.53	108.20
1	X	1775	A	P-O3'-C3'	17.83	141.10	119.70
1	X	1333	G	N3-C4-N9	-17.19	115.69	126.00
1	X	774	A	N7-C8-N9	16.88	122.24	113.80
1	X	540	G	P-O3'-C3'	16.87	139.94	119.70
1	X	1631	C	O4'-C1'-N1	16.27	121.21	108.20
1	X	537	C	O4'-C1'-N1	16.23	121.18	108.20
1	X	1333	G	O4'-C1'-N9	15.97	120.98	108.20
1	X	1288	A	O4'-C1'-N9	15.69	120.75	108.20
1	X	2497	A	P-O3'-C3'	15.66	138.49	119.70
1	X	1473	U	P-O3'-C3'	15.41	138.20	119.70
1	X	1631	C	P-O3'-C3'	15.28	138.03	119.70
1	X	2705	A	P-O3'-C3'	15.27	138.03	119.70
1	X	774	A	N1-C6-N6	15.10	127.66	118.60
1	X	1475	U	P-O3'-C3'	14.90	137.59	119.70
1	X	994	A	P-O3'-C3'	14.88	137.56	119.70
1	X	343	A	O4'-C1'-N9	14.77	120.02	108.20
1	X	1278	A	O4'-C1'-N9	14.74	120.00	108.20
1	X	777	A	P-O3'-C3'	14.73	137.37	119.70
1	X	2014	A	P-O3'-C3'	14.71	137.36	119.70
1	X	2706	U	P-O3'-C3'	14.71	137.35	119.70
1	X	399	G	P-O3'-C3'	14.67	137.30	119.70
1	X	774	A	C5-N7-C8	-14.57	96.61	103.90
1	X	1812	U	C1'-O4'-C4'	-14.53	98.27	109.90
1	X	540	G	N3-C4-N9	14.43	134.66	126.00
1	X	1249	G	P-O3'-C3'	14.41	136.99	119.70
1	X	1482	U	O4'-C1'-N1	14.39	119.71	108.20
1	X	802	A	P-O3'-C3'	14.30	136.86	119.70
1	X	100	G	P-O3'-C3'	13.66	136.10	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1409	U	P-O3'-C3'	13.51	135.91	119.70
1	X	176	A	P-O3'-C3'	13.47	135.86	119.70
1	X	2564	U	P-O3'-C3'	13.40	135.78	119.70
1	X	98	U	P-O3'-C3'	13.38	135.75	119.70
1	X	1570	C	O4'-C1'-N1	13.37	118.90	108.20
1	X	2736	U	P-O3'-C3'	13.23	135.58	119.70
1	X	774	A	C8-N9-C4	-13.23	100.51	105.80
1	X	774	A	C6-C5-N7	-13.06	123.16	132.30
1	X	1019	U	P-O3'-C3'	12.92	135.21	119.70
1	X	2404	A	P-O3'-C3'	12.91	135.20	119.70
1	X	1811	A	P-O3'-C3'	12.85	135.11	119.70
1	X	1820	G	P-O3'-C3'	12.84	135.11	119.70
1	X	1037	U	C1'-O4'-C4'	-12.83	99.63	109.90
1	X	1333	G	N3-C4-C5	12.79	135.00	128.60
1	X	540	G	N3-C2-N2	12.78	128.84	119.90
1	X	540	G	C4-C5-N7	12.77	115.91	110.80
1	X	1152	C	P-O3'-C3'	12.75	135.00	119.70
1	X	33	C	P-O3'-C3'	12.69	134.92	119.70
1	X	2018	G	P-O3'-C3'	12.67	134.91	119.70
1	X	1938	U	P-O3'-C3'	12.59	134.81	119.70
1	X	1561	A	P-O3'-C3'	12.59	134.80	119.70
1	X	1037	U	O4'-C1'-N1	12.53	118.22	108.20
1	X	2706	U	O4'-C1'-N1	12.51	118.21	108.20
1	X	1233	A	P-O3'-C3'	12.46	134.65	119.70
1	X	334	G	P-O3'-C3'	12.35	134.52	119.70
1	X	2371	A	O4'-C1'-N9	12.29	118.04	108.20
1	X	1467	U	P-O3'-C3'	-12.28	104.96	119.70
1	X	1963	G	P-O3'-C3'	12.27	134.42	119.70
1	X	469	G	O4'-C1'-N9	12.21	117.97	108.20
1	X	1055	A	P-O3'-C3'	12.18	134.31	119.70
1	X	467	U	C1'-O4'-C4'	-12.17	100.16	109.90
1	X	554	U	O4'-C1'-N1	12.06	117.84	108.20
1	X	1468	A	O4'-C1'-N9	12.06	117.84	108.20
1	X	1283	C	P-O3'-C3'	11.99	134.09	119.70
1	X	2770	A	P-O3'-C3'	11.98	134.07	119.70
1	X	683	A	P-O3'-C3'	11.94	134.03	119.70
1	X	1468	A	C8-N9-C4	-11.93	101.03	105.80
1	X	2608	A	P-O3'-C3'	11.85	133.92	119.70
1	X	2204	A	P-O3'-C3'	11.75	133.81	119.70
1	X	99	U	P-O3'-C3'	11.75	133.80	119.70
1	X	2312	A	P-O3'-C3'	11.72	133.77	119.70
1	X	1031	C	P-O3'-C3'	11.72	133.76	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1467	U	C5-C6-N1	11.71	128.56	122.70
1	X	774	A	C4-C5-N7	11.67	116.53	110.70
1	X	48	A	P-O3'-C3'	11.63	133.66	119.70
1	X	969	U	P-O3'-C3'	11.57	133.58	119.70
1	X	780	U	P-O3'-C3'	11.54	133.54	119.70
1	X	594	G	P-O3'-C3'	11.50	133.50	119.70
1	X	1790	G	P-O3'-C3'	11.48	133.48	119.70
2	Y	16	U	P-O3'-C3'	11.39	133.37	119.70
1	X	2589	C	P-O3'-C3'	11.37	133.34	119.70
1	X	1468	A	O4'-C1'-C2'	-11.17	94.63	105.80
1	X	2298	U	P-O3'-C3'	11.10	133.01	119.70
1	X	1975	G	P-O3'-C3'	11.09	133.01	119.70
1	X	2088	U	P-O3'-C3'	11.08	133.00	119.70
1	X	2498	U	P-O3'-C3'	11.08	132.99	119.70
1	X	1574	A	C4'-C3'-C2'	-11.06	91.54	102.60
1	X	514	G	P-O3'-C3'	11.05	132.96	119.70
1	X	537	C	N3-C2-O2	-11.05	114.17	121.90
1	X	2261	G	P-O3'-C3'	10.97	132.86	119.70
1	X	1333	G	C8-N9-C1'	10.96	141.25	127.00
1	X	1096	A	P-O3'-C3'	10.93	132.82	119.70
1	X	1574	A	O4'-C1'-N9	10.80	116.84	108.20
1	X	1669	A	O4'-C4'-C3'	-10.80	93.20	104.00
1	X	540	G	C6-C5-N7	-10.78	123.93	130.40
1	X	2596	C	O4'-C1'-N1	10.78	116.83	108.20
1	X	1186	G	P-O3'-C3'	10.71	132.55	119.70
1	X	656	U	O4'-C1'-N1	10.61	116.69	108.20
1	X	825	C	P-O3'-C3'	-10.58	107.01	119.70
1	X	1194	U	P-O3'-C3'	10.55	132.36	119.70
1	X	540	G	C5-C6-O6	-10.52	122.29	128.60
1	X	1688	U	N3-C4-O4	10.51	126.76	119.40
1	X	553	C	P-O3'-C3'	10.50	132.30	119.70
1	X	71	A	P-O3'-C3'	10.50	132.30	119.70
1	X	1850	G	P-O3'-C3'	10.48	132.28	119.70
1	X	664	C	P-O3'-C3'	10.47	132.27	119.70
1	X	1333	G	N3-C2-N2	-10.46	112.58	119.90
1	X	699	G	C5-N7-C8	-10.42	99.09	104.30
1	X	540	G	N3-C4-C5	-10.41	123.39	128.60
1	X	2551	A	P-O3'-C3'	10.37	132.15	119.70
1	X	342	G	P-O3'-C3'	10.37	132.14	119.70
1	X	537	C	C1'-O4'-C4'	-10.36	101.61	109.90
1	X	2769	C	C1'-O4'-C4'	-10.35	101.62	109.90
1	X	540	G	C5-C6-N1	10.34	116.67	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1496	G	P-O3'-C3'	10.31	132.07	119.70
1	X	458	G	P-O3'-C3'	10.29	132.05	119.70
1	X	939	C	C5'-C4'-O4'	10.29	121.45	109.10
1	X	518	A	P-O3'-C3'	10.27	132.02	119.70
1	X	814	G	O4'-C1'-N9	-10.25	100.00	108.20
1	X	1033	G	P-O3'-C3'	10.25	132.00	119.70
1	X	1053	G	P-O3'-C3'	10.19	131.93	119.70
1	X	542	A	C8-N9-C4	-10.17	101.73	105.80
1	X	540	G	C3'-C2'-C1'	10.15	109.62	101.50
1	X	1139	A	C1'-O4'-C4'	-10.13	101.80	109.90
1	X	803	C	P-O3'-C3'	10.09	131.81	119.70
1	X	83	A	P-O3'-C3'	10.08	131.79	119.70
1	X	2426	G	P-O3'-C3'	10.06	131.78	119.70
1	X	554	U	P-O3'-C3'	10.05	131.76	119.70
1	X	1632	A	P-O3'-C3'	10.01	131.71	119.70
1	X	2795	A	P-O3'-C3'	9.97	131.67	119.70
1	X	175	C	P-O3'-C3'	9.97	131.66	119.70
1	X	805	G	O4'-C1'-N9	-9.96	100.23	108.20
1	X	632	A	O4'-C1'-N9	9.93	116.14	108.20
1	X	2769	C	O4'-C1'-N1	9.90	116.12	108.20
1	X	1552	C	P-O3'-C3'	9.89	131.56	119.70
1	X	655	A	P-O3'-C3'	9.85	131.52	119.70
1	X	480	G	C5-C6-O6	-9.83	122.70	128.60
1	X	1812	U	O4'-C1'-N1	9.79	116.03	108.20
1	X	2418	A	P-O3'-C3'	9.78	131.43	119.70
1	X	1333	G	N9-C4-C5	9.76	109.31	105.40
1	X	1482	U	C1'-O4'-C4'	-9.76	102.09	109.90
1	X	814	G	P-O3'-C3'	9.75	131.40	119.70
1	X	2330	G	P-O3'-C3'	9.73	131.38	119.70
1	X	1442	C	P-O3'-C3'	9.72	131.36	119.70
1	X	2633	A	P-O3'-C3'	9.71	131.35	119.70
1	X	666	U	O4'-C1'-N1	9.67	115.94	108.20
1	X	558	G	P-O3'-C3'	9.66	131.30	119.70
1	X	73	A	P-O3'-C3'	9.66	131.29	119.70
1	X	2691	C	O4'-C1'-C2'	-9.66	96.14	105.80
1	X	1182	U	P-O3'-C3'	9.65	131.29	119.70
1	X	699	G	N3-C4-C5	9.63	133.42	128.60
1	X	759	C	C5-C6-N1	9.62	125.81	121.00
1	X	689	A	C5-N7-C8	-9.61	99.09	103.90
1	X	554	U	C1'-O4'-C4'	-9.61	102.22	109.90
1	X	1575	C	P-O3'-C3'	9.58	131.19	119.70
1	X	689	A	O4'-C1'-N9	9.56	115.85	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	3	U	P-O3'-C3'	9.55	131.16	119.70
1	X	542	A	C3'-C2'-C1'	9.55	109.14	101.50
1	X	1613	G	C1'-O4'-C4'	-9.54	102.27	109.90
1	X	691	C	O4'-C1'-N1	9.49	115.79	108.20
1	X	1333	G	C4-N9-C1'	-9.49	114.17	126.50
1	X	169	C	O4'-C1'-N1	9.48	115.79	108.20
1	X	542	A	N7-C8-N9	9.45	118.53	113.80
2	Y	26	G	P-O3'-C3'	9.43	131.02	119.70
1	X	1288	A	C3'-C2'-C1'	-9.40	93.98	101.50
1	X	841	G	O4'-C1'-N9	9.39	115.72	108.20
1	X	540	G	N7-C8-N9	9.39	117.79	113.10
1	X	2229	G	P-O3'-C3'	9.38	130.96	119.70
1	X	1288	A	O4'-C4'-C3'	-9.36	94.64	104.00
1	X	1664	G	O5'-P-OP2	9.35	121.92	110.70
1	X	1601	U	P-O3'-C3'	9.35	130.92	119.70
1	X	1975	G	C2'-C3'-O3'	9.35	130.07	109.50
1	X	1633	C	O4'-C1'-N1	9.28	115.63	108.20
1	X	1412	C	C3'-C2'-C1'	-9.28	94.08	101.50
1	X	2051	U	O4'-C1'-N1	9.23	115.58	108.20
1	X	1086	C	P-O3'-C3'	9.22	130.76	119.70
1	X	540	G	C5-N7-C8	-9.21	99.70	104.30
1	X	2669	C	N1-C2-O2	9.17	124.40	118.90
1	X	638	A	P-O3'-C3'	9.13	130.66	119.70
1	X	1689	U	O4'-C1'-N1	9.12	115.50	108.20
1	X	1345	G	P-O3'-C3'	9.12	130.64	119.70
1	X	2703	C	O4'-C1'-N1	9.10	115.48	108.20
1	X	699	G	N3-C4-N9	-9.09	120.55	126.00
1	X	1754	G	P-O3'-C3'	9.07	130.58	119.70
1	X	763	A	P-O3'-C3'	9.07	130.58	119.70
1	X	1459	U	P-O3'-C3'	9.06	130.58	119.70
1	X	467	U	O4'-C1'-N1	9.06	115.45	108.20
1	X	789	G	P-O3'-C3'	9.06	130.57	119.70
1	X	1574	A	C1'-O4'-C4'	-9.06	102.66	109.90
1	X	3	U	C3'-C2'-C1'	-9.03	94.27	101.50
1	X	2554	C	O4'-C1'-N1	9.01	115.41	108.20
1	X	666	U	C1'-O4'-C4'	-9.01	102.69	109.90
1	X	198	A	P-O3'-C3'	8.99	130.48	119.70
1	X	537	C	N1-C2-O2	8.99	124.29	118.90
1	X	1799	A	C1'-O4'-C4'	-8.97	102.72	109.90
1	X	1154	A	P-O3'-C3'	8.96	130.45	119.70
1	X	483	A	P-O3'-C3'	-8.95	108.96	119.70
1	X	2018	G	N3-C4-N9	-8.93	120.64	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2672	U	O4'-C1'-N1	8.93	115.34	108.20
1	X	796	A	C5-N7-C8	-8.92	99.44	103.90
1	X	1184	G	P-O3'-C3'	8.91	130.39	119.70
1	X	515	A	P-O3'-C3'	8.89	130.37	119.70
1	X	1137	A	P-O3'-C3'	8.89	130.37	119.70
1	X	2222	U	O4'-C1'-N1	8.89	115.31	108.20
1	X	2018	G	N9-C1'-C2'	8.86	125.52	114.00
1	X	341	A	P-O3'-C3'	8.84	130.31	119.70
1	X	2475	C	O4'-C1'-N1	8.82	115.26	108.20
1	X	574	C	O4'-C1'-N1	8.82	115.26	108.20
1	X	1830	C	P-O3'-C3'	8.82	130.28	119.70
1	X	2671	C	O4'-C1'-N1	8.82	115.25	108.20
1	X	689	A	N7-C8-N9	8.81	118.20	113.80
1	X	559	C	N1-C1'-C2'	8.80	125.44	114.00
1	X	2706	U	C4'-C3'-C2'	8.78	111.38	102.60
1	X	1746	A	O4'-C1'-N9	8.78	115.23	108.20
1	X	2689	C	P-O3'-C3'	8.78	130.24	119.70
1	X	418	C	C1'-O4'-C4'	-8.75	102.90	109.90
1	X	774	A	C5-C6-N1	-8.74	113.33	117.70
1	X	841	G	C8-N9-C4	-8.74	102.90	106.40
1	X	1812	U	N1-C1'-C2'	8.73	125.34	114.00
1	X	1509	A	O4'-C1'-N9	8.72	115.17	108.20
1	X	1265	G	O4'-C1'-N9	-8.70	101.24	108.20
1	X	2782	G	C5-C6-O6	-8.70	123.38	128.60
1	X	686	C	O4'-C1'-N1	8.70	115.16	108.20
1	X	483	A	O4'-C1'-N9	8.68	115.14	108.20
1	X	1278	A	C3'-C2'-C1'	-8.65	94.58	101.50
1	X	540	G	N9-C4-C5	-8.65	101.94	105.40
1	X	625	A	P-O3'-C3'	8.64	130.07	119.70
1	X	1656	U	O4'-C1'-N1	8.64	115.11	108.20
1	X	1468	A	P-O3'-C3'	8.62	130.04	119.70
1	X	566	U	O4'-C1'-N1	8.61	115.08	108.20
1	X	758	G	C2'-C3'-O3'	8.60	128.43	109.50
1	X	540	G	N1-C2-N2	-8.59	108.47	116.20
1	X	953	G	O4'-C1'-N9	8.59	115.07	108.20
1	X	804	C	O4'-C1'-N1	8.58	115.07	108.20
1	X	2691	C	P-O3'-C3'	8.58	130.00	119.70
1	X	656	U	P-O3'-C3'	8.58	130.00	119.70
1	X	1938	U	C4'-C3'-C2'	8.58	111.18	102.60
1	X	216	U	O4'-C1'-N1	8.58	115.06	108.20
1	X	467	U	P-O3'-C3'	8.57	129.98	119.70
1	X	490	A	O4'-C1'-N9	8.56	115.05	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	54	U	O4'-C1'-N1	8.56	115.05	108.20
1	X	204	A	P-O3'-C3'	8.55	129.96	119.70
1	X	242	A	C4'-C3'-C2'	-8.55	94.05	102.60
1	X	788	G	P-O3'-C3'	8.53	129.93	119.70
1	X	1223	G	C3'-C2'-C1'	8.52	108.31	101.50
1	X	1399	C	O4'-C1'-N1	8.51	115.01	108.20
1	X	181	A	P-O3'-C3'	8.50	129.90	119.70
1	X	1974	U	O4'-C1'-N1	8.49	115.00	108.20
1	X	2594	U	C5-C6-N1	8.45	126.93	122.70
1	X	1602	G	P-O3'-C3'	8.45	129.84	119.70
1	X	1467	U	C4-C5-C6	-8.44	114.64	119.70
1	X	1278	A	C1'-O4'-C4'	-8.43	103.16	109.90
1	X	939	C	C1'-O4'-C4'	-8.42	103.16	109.90
1	X	1581	C	P-O3'-C3'	8.42	129.80	119.70
1	X	343	A	C8-N9-C4	-8.41	102.44	105.80
1	X	31	C	O4'-C1'-N1	8.40	114.92	108.20
1	X	2426	G	O4'-C1'-N9	8.40	114.92	108.20
1	X	537	C	N3-C4-N4	-8.38	112.13	118.00
1	X	1716	G	C4'-C3'-C2'	8.38	110.98	102.60
1	X	1441	A	P-O3'-C3'	8.37	129.75	119.70
1	X	2778	U	P-O3'-C3'	8.37	129.74	119.70
1	X	1469	U	N1-C1'-C2'	8.34	124.85	114.00
1	X	1574	A	C5'-C4'-O4'	8.34	119.11	109.10
1	X	2189	A	P-O3'-C3'	8.33	129.69	119.70
1	X	1953	A	P-O5'-C5'	-8.32	107.58	120.90
1	X	2018	G	C5'-C4'-C3'	-8.32	102.69	116.00
1	X	2685	A	N1-C6-N6	-8.32	113.61	118.60
1	X	1539	U	O4'-C1'-N1	8.31	114.85	108.20
1	X	1753	A	O4'-C1'-N9	8.30	114.84	108.20
1	X	2408	G	P-O5'-C5'	-8.30	107.62	120.90
1	X	2018	G	N3-C4-C5	8.30	132.75	128.60
1	X	2745	A	P-O3'-C3'	8.29	129.65	119.70
1	X	346	C	C6-N1-C2	-8.29	116.98	120.30
1	X	2191	A	O4'-C1'-N9	8.28	114.83	108.20
1	X	2867	G	N7-C8-N9	8.28	117.24	113.10
1	X	809	C	O4'-C1'-N1	8.27	114.82	108.20
1	X	2867	G	C5-N7-C8	-8.27	100.17	104.30
1	X	841	G	N7-C8-N9	8.26	117.23	113.10
1	X	358	C	O4'-C1'-N1	8.26	114.81	108.20
1	X	631	G	P-O5'-C5'	-8.25	107.70	120.90
1	X	346	C	O4'-C1'-N1	8.24	114.79	108.20
1	X	467	U	C2-N1-C1'	8.21	127.56	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	490	A	P-O3'-C3'	8.21	129.55	119.70
1	X	731	A	P-O3'-C3'	8.20	129.54	119.70
1	X	2710	C	P-O3'-C3'	-8.20	109.86	119.70
1	X	1523	A	P-O3'-C3'	8.20	129.53	119.70
1	X	1765	C	N1-C2-O2	8.19	123.81	118.90
1	X	1251	G	O4'-C1'-N9	8.18	114.75	108.20
1	X	2824	C	P-O3'-C3'	8.18	129.51	119.70
1	X	2491	C	O5'-P-OP2	-8.18	98.34	105.70
1	X	847	C	O4'-C1'-N1	8.17	114.74	108.20
1	X	593	C	O4'-C1'-N1	8.15	114.72	108.20
1	X	661	C	N1-C2-O2	8.15	123.79	118.90
1	X	2857	C	O4'-C1'-N1	8.12	114.69	108.20
1	X	469	G	P-O3'-C3'	8.12	129.44	119.70
1	X	2034	A	P-O3'-C3'	8.11	129.44	119.70
1	X	2867	G	C4-C5-N7	8.11	114.04	110.80
1	X	2487	G	O4'-C1'-N9	8.10	114.68	108.20
1	X	2730	A	P-O3'-C3'	8.10	129.42	119.70
1	X	1188	A	P-O3'-C3'	8.09	129.41	119.70
1	X	2298	U	O4'-C1'-N1	8.09	114.67	108.20
1	X	751	G	O4'-C4'-C3'	-8.08	95.92	104.00
1	X	597	U	O4'-C4'-C3'	-8.07	95.93	104.00
1	X	1232	U	O4'-C1'-N1	8.07	114.66	108.20
1	X	1712	G	N3-C2-N2	8.06	125.54	119.90
1	X	758	G	C3'-C2'-C1'	-8.06	95.05	101.50
1	X	1310	C	O4'-C1'-N1	8.05	114.64	108.20
1	X	1962	C	C3'-C2'-C1'	-8.05	95.06	101.50
1	X	99	U	O4'-C1'-N1	8.05	114.64	108.20
1	X	813	A	P-O3'-C3'	8.05	129.36	119.70
1	X	859	U	O4'-C1'-N1	8.05	114.64	108.20
1	X	526	C	O4'-C1'-N1	8.04	114.64	108.20
1	X	580	A	P-O3'-C3'	8.04	129.35	119.70
1	X	39	C	O4'-C1'-N1	8.03	114.62	108.20
1	X	1524	C	P-O3'-C3'	8.02	129.32	119.70
1	X	2667	C	P-O3'-C3'	8.02	129.32	119.70
1	X	739	G	O4'-C1'-N9	8.01	114.61	108.20
1	X	74	G	O4'-C4'-C3'	-8.00	96.00	104.00
1	X	542	A	N1-C2-N3	8.00	133.30	129.30
1	X	1468	A	C5-C6-N1	7.99	121.70	117.70
1	X	1710	U	P-O3'-C3'	7.99	129.29	119.70
1	X	117	A	P-O3'-C3'	7.99	129.28	119.70
1	X	313	U	O4'-C1'-N1	7.96	114.57	108.20
1	X	2854	G	C1'-O4'-C4'	-7.96	103.53	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2854	G	P-O3'-C3'	7.96	129.25	119.70
1	X	2859	U	O4'-C1'-N1	7.95	114.56	108.20
1	X	579	G	C4-C5-N7	-7.94	107.62	110.80
1	X	1314	A	P-O3'-C3'	7.94	129.22	119.70
1	X	542	A	C6-N1-C2	-7.93	113.84	118.60
1	X	1673	C	O4'-C1'-N1	7.93	114.54	108.20
1	X	2492	G	O4'-C1'-N9	7.93	114.54	108.20
1	X	1469	U	P-O3'-C3'	7.91	129.19	119.70
1	X	796	A	N1-C6-N6	7.91	123.35	118.60
1	X	841	G	N9-C1'-C2'	7.91	124.28	114.00
1	X	685	U	O4'-C1'-N1	7.90	114.52	108.20
1	X	165	G	O4'-C1'-N9	7.90	114.52	108.20
1	X	1139	A	O4'-C1'-N9	7.89	114.52	108.20
1	X	631	G	P-O3'-C3'	7.89	129.17	119.70
1	X	467	U	C4'-C3'-C2'	-7.89	94.71	102.60
1	X	699	G	N7-C8-N9	7.88	117.04	113.10
1	X	236	C	O4'-C1'-N1	7.88	114.50	108.20
1	X	2018	G	O4'-C1'-N9	7.87	114.50	108.20
1	X	100	G	O4'-C1'-N9	7.87	114.49	108.20
1	X	2258	G	C1'-O4'-C4'	-7.86	103.61	109.90
1	X	1679	U	N3-C2-O2	-7.85	116.70	122.20
1	X	307	C	O4'-C1'-N1	7.85	114.48	108.20
1	X	2009	U	O4'-C1'-N1	7.84	114.48	108.20
1	X	2810	A	P-O3'-C3'	7.84	129.11	119.70
1	X	554	U	N1-C1'-C2'	7.84	124.19	114.00
2	Y	42	U	O4'-C1'-N1	7.84	114.47	108.20
1	X	774	A	C5-C6-N6	-7.83	117.43	123.70
1	X	1775	A	C2'-C3'-O3'	7.83	126.73	109.50
1	X	1770	U	O4'-C4'-C3'	-7.83	96.17	104.00
1	X	1526	U	O4'-C1'-N1	7.82	114.46	108.20
1	X	2854	G	N9-C1'-C2'	7.82	124.16	114.00
1	X	868	U	O4'-C1'-N1	7.81	114.45	108.20
1	X	308	C	O4'-C1'-N1	7.81	114.45	108.20
1	X	864	C	O4'-C1'-N1	7.81	114.45	108.20
1	X	1161	U	O4'-C1'-N1	7.80	114.44	108.20
1	X	672	C	O4'-C4'-C3'	-7.80	96.20	104.00
1	X	1688	U	N3-C4-C5	-7.80	109.92	114.60
13	K	94	TYR	C-N-CA	7.79	141.19	121.70
1	X	2597	G	O4'-C1'-N9	7.78	114.42	108.20
1	X	2489	C	O4'-C1'-N1	7.78	114.42	108.20
1	X	2275	U	P-O3'-C3'	7.77	129.02	119.70
1	X	577	U	N3-C4-C5	-7.77	109.94	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1496	G	C3'-C2'-C1'	-7.76	95.29	101.50
1	X	2299	A	P-O3'-C3'	7.76	129.02	119.70
1	X	956	A	N1-C6-N6	7.75	123.25	118.60
1	X	1467	U	N1-C2-N3	-7.74	110.26	114.90
1	X	2043	A	O4'-C1'-N9	7.73	114.39	108.20
1	X	242	A	C1'-O4'-C4'	-7.73	103.72	109.90
1	X	312	G	P-O3'-C3'	7.72	128.97	119.70
1	X	526	C	C3'-C2'-C1'	-7.72	95.32	101.50
1	X	1829	C	O4'-C1'-N1	7.71	114.37	108.20
1	X	927	C	O4'-C1'-N1	7.70	114.36	108.20
1	X	1844	C	O4'-C1'-N1	7.68	114.35	108.20
1	X	1947	G	P-O3'-C3'	7.67	128.91	119.70
1	X	2813	G	O4'-C1'-N9	7.67	114.34	108.20
1	X	2062	U	O4'-C1'-N1	7.67	114.33	108.20
1	X	1561	A	C3'-C2'-C1'	-7.66	95.37	101.50
1	X	841	G	O4'-C4'-C3'	-7.66	96.34	104.00
1	X	462	G	C5-C6-N1	-7.66	107.67	111.50
1	X	1663	C	N1-C2-O2	7.64	123.49	118.90
1	X	1141	U	C2'-C3'-O3'	7.64	126.31	109.50
1	X	1674	C	O4'-C1'-N1	7.64	114.31	108.20
1	X	2501	U	C5'-C4'-C3'	-7.63	103.80	116.00
1	X	2018	G	C5-N7-C8	-7.62	100.49	104.30
1	X	2756	A	P-O3'-C3'	7.62	128.85	119.70
1	X	537	C	P-O3'-C3'	7.61	128.83	119.70
1	X	1976	U	P-O5'-C5'	-7.60	108.73	120.90
19	Q	60	GLY	C-N-CA	7.60	140.70	121.70
1	X	480	G	C4-C5-N7	7.59	113.84	110.80
1	X	1392	U	P-O3'-C3'	7.59	128.81	119.70
1	X	1468	A	C3'-C2'-C1'	-7.59	95.43	101.50
1	X	2000	U	O5'-P-OP2	-7.59	98.87	105.70
1	X	1279	G	C5-C6-O6	-7.58	124.05	128.60
1	X	2808	U	C1'-O4'-C4'	-7.57	103.84	109.90
1	X	2016	A	P-O3'-C3'	7.57	128.78	119.70
1	X	768	U	O4'-C1'-N1	7.57	114.25	108.20
1	X	1333	G	C8-N9-C4	-7.56	103.38	106.40
1	X	1607	A	P-O3'-C3'	7.56	128.77	119.70
1	X	1364	C	O4'-C1'-N1	7.55	114.24	108.20
1	X	699	G	C4-C5-N7	7.55	113.82	110.80
1	X	796	A	N7-C8-N9	7.55	117.58	113.80
1	X	2005	U	O4'-C1'-N1	7.54	114.24	108.20
1	X	1072	U	P-O3'-C3'	7.54	128.75	119.70
1	X	312	G	C1'-O4'-C4'	-7.54	103.87	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	246	C	O4'-C1'-N1	7.54	114.23	108.20
2	Y	30	C	O4'-C1'-N1	7.54	114.23	108.20
1	X	1963	G	C2'-C3'-O3'	7.53	126.08	109.50
1	X	2550	C	O4'-C1'-N1	7.53	114.22	108.20
1	X	1562	G	O4'-C1'-N9	7.51	114.21	108.20
1	X	520	C	P-O3'-C3'	7.51	128.71	119.70
1	X	2477	C	C5'-C4'-O4'	-7.50	100.10	109.10
1	X	759	C	C6-N1-C2	-7.49	117.31	120.30
1	X	2824	C	C2'-C3'-O3'	7.49	125.97	109.50
1	X	1466	C	C4'-C3'-C2'	-7.48	95.12	102.60
1	X	2370	G	C1'-O4'-C4'	-7.48	103.92	109.90
1	X	3	U	C2'-C3'-O3'	7.48	125.95	109.50
1	X	456	C	O4'-C1'-N1	7.48	114.18	108.20
1	X	774	A	C2-N3-C4	-7.48	106.86	110.60
1	X	1306	U	O4'-C1'-N1	7.48	114.18	108.20
1	X	418	C	C5'-C4'-O4'	7.46	118.05	109.10
1	X	1128	G	P-O3'-C3'	7.45	128.64	119.70
1	X	2031	A	O4'-C1'-N9	7.44	114.16	108.20
1	X	661	C	C4'-C3'-C2'	-7.44	95.16	102.60
1	X	1467	U	N1-C2-O2	7.44	128.01	122.80
1	X	408	U	P-O3'-C3'	7.43	128.62	119.70
1	X	394	U	O4'-C1'-N1	7.42	114.14	108.20
1	X	218	A	P-O3'-C3'	7.42	128.61	119.70
1	X	939	C	O4'-C1'-N1	7.41	114.13	108.20
1	X	2206	C	O4'-C1'-N1	7.41	114.13	108.20
1	X	346	C	N1-C1'-C2'	7.41	123.63	114.00
1	X	1917	C	O4'-C1'-N1	7.41	114.13	108.20
1	X	1770	U	N3-C2-O2	-7.41	117.02	122.20
1	X	1429	A	C1'-O4'-C4'	-7.39	103.98	109.90
1	X	1988	A	P-O3'-C3'	7.39	128.57	119.70
1	X	503	G	O4'-C4'-C3'	-7.39	96.61	104.00
1	X	509	U	O4'-C1'-N1	7.38	114.11	108.20
1	X	796	A	C2-N3-C4	-7.38	106.91	110.60
1	X	537	C	C5-C6-N1	-7.38	117.31	121.00
1	X	429	C	O4'-C1'-N1	7.37	114.09	108.20
1	X	2193	C	O4'-C1'-N1	7.36	114.09	108.20
1	X	357	A	P-O3'-C3'	7.36	128.53	119.70
1	X	2392	G	O4'-C1'-N9	7.36	114.08	108.20
1	X	938	G	O4'-C1'-N9	7.35	114.08	108.20
1	X	1034	U	O4'-C1'-N1	7.35	114.08	108.20
1	X	826	U	O4'-C1'-N1	7.34	114.07	108.20
1	X	1265	G	P-O5'-C5'	7.34	132.64	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1656	U	P-O3'-C3'	7.34	128.50	119.70
1	X	68	C	O4'-C1'-N1	7.33	114.07	108.20
1	X	1336	G	C5-C6-O6	-7.33	124.20	128.60
1	X	192	G	P-O3'-C3'	7.33	128.50	119.70
1	X	838	A	OP1-P-O3'	7.33	121.31	105.20
1	X	89	A	P-O3'-C3'	7.32	128.49	119.70
1	X	765	C	P-O3'-C3'	7.32	128.48	119.70
1	X	2270	U	O4'-C1'-N1	7.32	114.06	108.20
2	Y	81	C	O4'-C1'-N1	7.32	114.05	108.20
1	X	174	A	P-O3'-C3'	7.31	128.48	119.70
1	X	2395	C	O4'-C1'-N1	7.30	114.04	108.20
1	X	777	A	C2'-C3'-O3'	7.29	125.53	109.50
1	X	1593	C	O4'-C1'-N1	7.29	114.03	108.20
1	X	2752	C	O4'-C1'-N1	7.29	114.03	108.20
1	X	1068	A	P-O3'-C3'	7.28	128.44	119.70
1	X	1470	G	P-O3'-C3'	-7.28	110.97	119.70
1	X	1044	U	P-O3'-C3'	7.27	128.43	119.70
1	X	661	C	O4'-C1'-N1	7.26	114.01	108.20
1	X	1339	U	O4'-C1'-N1	7.26	114.01	108.20
1	X	661	C	N3-C2-O2	-7.26	116.82	121.90
1	X	926	C	O4'-C1'-N1	7.25	114.00	108.20
1	X	1334	A	O4'-C4'-C3'	-7.25	96.75	104.00
1	X	343	A	N7-C8-N9	7.24	117.42	113.80
1	X	2589	C	O4'-C1'-N1	-7.24	102.41	108.20
1	X	1770	U	C5-C6-N1	-7.24	119.08	122.70
1	X	59	G	P-O3'-C3'	7.23	128.37	119.70
1	X	742	G	P-O3'-C3'	7.22	128.37	119.70
1	X	1670	G	P-O3'-C3'	7.22	128.37	119.70
1	X	418	C	O4'-C1'-N1	7.22	113.98	108.20
1	X	2185	U	O4'-C1'-N1	7.22	113.97	108.20
1	X	2853	U	O4'-C1'-N1	7.21	113.97	108.20
1	X	1680	U	O4'-C4'-C3'	-7.21	96.79	104.00
1	X	882	C	O4'-C1'-N1	7.21	113.97	108.20
1	X	947	C	O4'-C1'-N1	7.21	113.96	108.20
1	X	1447	U	O4'-C1'-N1	7.20	113.96	108.20
1	X	2408	G	C5'-C4'-C3'	-7.20	104.47	116.00
1	X	843	G	P-O3'-C3'	7.20	128.34	119.70
1	X	518	A	N9-C1'-C2'	7.19	123.35	114.00
1	X	1333	G	C2-N3-C4	-7.19	108.31	111.90
1	X	1474	A	P-O3'-C3'	7.17	128.31	119.70
1	X	525	A	O4'-C1'-N9	7.17	113.94	108.20
1	X	1812	U	P-O3'-C3'	7.17	128.31	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	387	A	P-O3'-C3'	7.17	128.31	119.70
1	X	824	U	N1-C1'-C2'	7.16	123.31	114.00
1	X	2782	G	N1-C6-O6	7.16	124.19	119.90
1	X	1277	G	O4'-C1'-N9	7.15	113.92	108.20
1	X	514	G	O4'-C1'-N9	-7.14	102.48	108.20
1	X	2731	G	P-O3'-C3'	7.14	128.27	119.70
1	X	2668	U	C5-C4-O4	7.14	130.18	125.90
1	X	242	A	O4'-C4'-C3'	-7.14	96.86	104.00
1	X	517	A	P-O3'-C3'	7.14	128.26	119.70
1	X	1664	G	O5'-P-OP1	-7.14	99.28	105.70
1	X	2708	U	O4'-C1'-N1	7.14	113.91	108.20
1	X	1570	C	C1'-O4'-C4'	-7.13	104.19	109.90
1	X	714	G	O4'-C4'-C3'	-7.13	96.87	104.00
1	X	801	A	P-O3'-C3'	7.13	128.25	119.70
1	X	2217	G	P-O3'-C3'	7.13	128.25	119.70
1	X	2615	U	O4'-C1'-N1	7.13	113.90	108.20
1	X	1266	G	P-O3'-C3'	7.12	128.25	119.70
1	X	2744	A	O4'-C1'-N9	7.12	113.90	108.20
1	X	1467	U	C4'-C3'-O3'	7.12	127.24	113.00
1	X	540	G	C4-N9-C1'	7.12	135.75	126.50
1	X	542	A	C6-C5-N7	-7.12	127.32	132.30
1	X	1679	U	O4'-C4'-C3'	-7.12	96.88	104.00
1	X	1355	A	P-O3'-C3'	7.12	128.24	119.70
1	X	2408	G	C4'-C3'-C2'	7.12	109.72	102.60
1	X	617	U	N3-C2-O2	-7.10	117.23	122.20
1	X	2553	G	C5-C6-O6	-7.10	124.34	128.60
1	X	2808	U	C3'-C2'-C1'	-7.09	95.83	101.50
1	X	780	U	O4'-C1'-N1	7.09	113.87	108.20
1	X	1442	C	N1-C2-O2	7.09	123.15	118.90
1	X	494	A	N9-C1'-C2'	-7.08	104.21	112.00
1	X	1594	U	O4'-C1'-N1	7.07	113.86	108.20
1	X	1652	G	O4'-C1'-N9	-7.07	102.54	108.20
1	X	2485	U	O4'-C1'-N1	7.07	113.86	108.20
2	Y	17	A	O4'-C1'-N9	7.07	113.86	108.20
1	X	491	A	O4'-C1'-N9	-7.07	102.55	108.20
1	X	2872	U	O4'-C1'-N1	7.06	113.85	108.20
1	X	2808	U	C5'-C4'-O4'	7.06	117.57	109.10
1	X	1333	G	N1-C2-N2	7.06	122.55	116.20
1	X	537	C	C5'-C4'-O4'	7.06	117.57	109.10
1	X	2722	C	O4'-C1'-N1	7.05	113.84	108.20
1	X	1221	C	O4'-C1'-N1	7.05	113.84	108.20
1	X	666	U	P-O3'-C3'	7.05	128.16	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	711	C	O4'-C1'-N1	7.05	113.84	108.20
1	X	1742	G	P-O3'-C3'	-7.05	111.24	119.70
1	X	1986	G	P-O3'-C3'	-7.04	111.25	119.70
1	X	2626	U	O4'-C1'-N1	7.04	113.84	108.20
1	X	2830	U	O4'-C1'-N1	7.04	113.83	108.20
1	X	1200	G	O4'-C1'-N9	7.04	113.83	108.20
1	X	1634	A	P-O3'-C3'	7.04	128.15	119.70
1	X	1651	U	O4'-C1'-N1	7.04	113.83	108.20
1	X	1935	A	P-O3'-C3'	7.04	128.15	119.70
1	X	845	U	O4'-C1'-N1	7.03	113.82	108.20
1	X	1302	C	O4'-C1'-N1	7.03	113.82	108.20
1	X	453	U	O4'-C1'-N1	7.02	113.82	108.20
1	X	761	G	C1'-O4'-C4'	-7.02	104.28	109.90
1	X	937	C	O4'-C1'-N1	7.02	113.82	108.20
1	X	227	G	O4'-C1'-N9	7.02	113.81	108.20
1	X	469	G	N3-C4-C5	-7.02	125.09	128.60
1	X	1071	U	P-O3'-C3'	7.01	128.11	119.70
1	X	2864	C	O4'-C1'-N1	7.01	113.81	108.20
1	X	1776	A	P-O3'-C3'	7.00	128.10	119.70
1	X	2669	C	O4'-C1'-C2'	-7.00	98.81	105.80
1	X	1946	U	N3-C2-O2	-6.99	117.31	122.20
1	X	1434	U	P-O3'-C3'	6.99	128.09	119.70
1	X	2039	G	C8-N9-C4	-6.97	103.61	106.40
1	X	592	G	O4'-C1'-N9	6.97	113.78	108.20
1	X	117	A	C1'-O4'-C4'	-6.97	104.33	109.90
1	X	474	G	O4'-C1'-N9	6.96	113.77	108.20
1	X	485	G	P-O3'-C3'	6.96	128.06	119.70
1	X	2698	G	C4'-C3'-C2'	-6.96	95.64	102.60
1	X	459	A	P-O3'-C3'	6.95	128.04	119.70
1	X	1434	U	C1'-O4'-C4'	-6.95	104.34	109.90
1	X	304	A	P-O5'-C5'	6.94	132.01	120.90
1	X	1550	C	O4'-C1'-N1	6.94	113.75	108.20
1	X	1997	A	N1-C6-N6	6.93	122.76	118.60
1	X	1434	U	O4'-C1'-N1	6.93	113.75	108.20
1	X	1663	C	OP1-P-O3'	6.93	120.45	105.20
1	X	835	U	N3-C2-O2	-6.93	117.35	122.20
1	X	2347	C	O4'-C1'-N1	6.93	113.74	108.20
1	X	2788	C	O4'-C1'-N1	6.92	113.74	108.20
1	X	751	G	C2'-C3'-O3'	6.92	124.78	113.70
1	X	1412	C	P-O3'-C3'	6.92	128.00	119.70
1	X	594	G	O4'-C1'-N9	6.92	113.73	108.20
1	X	1094	C	O4'-C1'-N1	6.91	113.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2581	A	P-O3'-C3'	6.91	127.99	119.70
1	X	467	U	C6-N1-C1'	-6.91	111.53	121.20
2	Y	37	C	O4'-C1'-N1	6.91	113.72	108.20
1	X	526	C	O5'-P-OP2	-6.90	99.49	105.70
1	X	1712	G	N3-C4-N9	6.90	130.14	126.00
1	X	308	C	P-O5'-C5'	6.90	131.94	120.90
1	X	2660	C	O4'-C1'-N1	6.90	113.72	108.20
1	X	2088	U	O4'-C1'-N1	6.90	113.72	108.20
1	X	1984	A	P-O5'-C5'	-6.89	109.87	120.90
1	X	2018	G	P-O5'-C5'	-6.89	109.87	120.90
1	X	585	U	O4'-C1'-N1	6.89	113.71	108.20
1	X	190	A	O4'-C1'-N9	6.89	113.71	108.20
1	X	305	A	O4'-C1'-N9	6.89	113.71	108.20
1	X	206	U	O4'-C1'-N1	6.88	113.71	108.20
13	K	7	GLY	C-N-CA	6.88	138.91	121.70
1	X	1865	C	O4'-C1'-N1	6.88	113.70	108.20
1	X	2043	A	P-O3'-C3'	6.88	127.95	119.70
1	X	2067	U	O4'-C1'-N1	6.87	113.70	108.20
1	X	413	G	C8-N9-C4	-6.86	103.66	106.40
1	X	650	U	O4'-C1'-N1	6.86	113.69	108.20
9	G	106	TYR	N-CA-CB	6.85	122.94	110.60
1	X	2075	U	P-O3'-C3'	6.85	127.92	119.70
1	X	469	G	C1'-O4'-C4'	-6.85	104.42	109.90
1	X	2523	G	O4'-C1'-N9	6.84	113.67	108.20
1	X	1432	G	O4'-C1'-N9	6.84	113.67	108.20
1	X	1249	G	C4'-C3'-C2'	6.84	109.44	102.60
1	X	334	G	C1'-O4'-C4'	-6.84	104.43	109.90
1	X	430	C	O4'-C1'-N1	6.84	113.67	108.20
1	X	2407	G	P-O3'-C3'	6.83	127.90	119.70
1	X	2423	G	O5'-P-OP2	-6.83	99.55	105.70
1	X	1680	U	O5'-P-OP2	-6.81	99.57	105.70
1	X	840	U	O4'-C1'-N1	6.81	113.65	108.20
1	X	796	A	C4-C5-N7	6.81	114.10	110.70
1	X	2208	U	O4'-C1'-N1	6.80	113.64	108.20
1	X	2799	C	O4'-C1'-N1	6.80	113.64	108.20
1	X	2082	C	O4'-C1'-N1	6.80	113.64	108.20
1	X	92	U	O4'-C1'-N1	6.79	113.63	108.20
1	X	2774	U	O4'-C1'-N1	6.79	113.63	108.20
1	X	539	A	C1'-O4'-C4'	-6.79	104.47	109.90
1	X	556	A	P-O3'-C3'	6.79	127.84	119.70
1	X	1787	U	O4'-C1'-N1	6.78	113.63	108.20
1	X	689	A	C2-N3-C4	-6.78	107.21	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	689	A	C4-C5-N7	6.78	114.09	110.70
2	Y	57	U	O4'-C1'-N1	6.78	113.62	108.20
1	X	1223	G	C6-C5-N7	-6.78	126.33	130.40
1	X	1771	A	P-O3'-C3'	6.77	127.83	119.70
1	X	2236	U	O4'-C1'-N1	6.77	113.62	108.20
1	X	1093	U	O4'-C1'-N1	6.77	113.61	108.20
1	X	1010	U	P-O5'-C5'	6.76	131.72	120.90
1	X	2671	C	O5'-P-OP2	-6.75	99.62	105.70
1	X	333	A	P-O3'-C3'	6.75	127.80	119.70
1	X	1279	G	C4-C5-N7	6.75	113.50	110.80
1	X	2038	C	OP2-P-O3'	6.75	120.05	105.20
1	X	2456	U	O4'-C1'-N1	6.75	113.60	108.20
1	X	759	C	C4'-C3'-C2'	6.75	109.34	102.60
1	X	730	C	P-O3'-C3'	6.74	127.79	119.70
1	X	1344	C	N1-C2-O2	6.74	122.94	118.90
1	X	943	U	O4'-C1'-N1	6.74	113.59	108.20
2	Y	55	C	O4'-C1'-N1	6.74	113.59	108.20
1	X	2408	G	C8-N9-C4	-6.74	103.70	106.40
1	X	1946	U	N1-C2-O2	6.73	127.51	122.80
1	X	981	C	O4'-C1'-N1	6.73	113.58	108.20
1	X	995	A	O4'-C1'-N9	6.73	113.58	108.20
1	X	1922	U	P-O3'-C3'	6.73	127.77	119.70
1	X	1664	G	P-O5'-C5'	6.73	131.66	120.90
1	X	1862	C	O4'-C1'-N1	6.73	113.58	108.20
1	X	1958	G	O4'-C4'-C3'	-6.71	97.29	104.00
1	X	1947	G	O4'-C1'-N9	-6.71	102.83	108.20
2	Y	16	U	N1-C1'-C2'	6.71	122.72	114.00
1	X	1522	C	C3'-C2'-C1'	-6.71	96.14	101.50
1	X	866	U	O4'-C1'-N1	6.70	113.56	108.20
1	X	1314	A	C4'-C3'-O3'	-6.70	95.33	109.40
1	X	1731	C	O4'-C1'-N1	6.70	113.56	108.20
1	X	2373	C	O4'-C1'-N1	6.70	113.56	108.20
1	X	418	C	C4'-C3'-C2'	-6.70	95.90	102.60
1	X	519	C	C6-N1-C2	-6.70	117.62	120.30
1	X	774	A	C6-N1-C2	6.70	122.62	118.60
1	X	1712	G	O4'-C1'-N9	6.69	113.55	108.20
1	X	632	A	P-O3'-C3'	6.69	127.73	119.70
1	X	1319	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	1662	G	P-O3'-C3'	6.69	127.72	119.70
1	X	2478	C	O4'-C1'-N1	6.69	113.55	108.20
1	X	948	C	P-O3'-C3'	-6.68	111.68	119.70
1	X	951	G	C3'-C2'-C1'	-6.68	96.15	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1804	U	O4'-C1'-N1	6.67	113.54	108.20
1	X	564	U	O4'-C1'-N1	6.67	113.54	108.20
1	X	1183	C	O4'-C1'-N1	6.67	113.53	108.20
1	X	2480	C	O4'-C1'-N1	6.67	113.53	108.20
1	X	533	C	O4'-C1'-N1	6.65	113.52	108.20
1	X	343	A	N9-C1'-C2'	6.65	122.65	114.00
1	X	1468	A	N7-C8-N9	6.65	117.13	113.80
1	X	2189	A	C8-N9-C4	-6.64	103.14	105.80
1	X	928	G	C5-C6-O6	-6.64	124.61	128.60
1	X	494	A	C3'-C2'-C1'	6.64	106.81	101.50
1	X	2501	U	O4'-C1'-N1	6.64	113.51	108.20
1	X	646	C	O4'-C1'-N1	6.64	113.51	108.20
1	X	1980	A	C5'-C4'-O4'	6.63	117.06	109.10
1	X	1712	G	N1-C2-N2	-6.63	110.24	116.20
1	X	1725	C	O4'-C1'-N1	6.62	113.50	108.20
1	X	35	G	O4'-C1'-N9	6.62	113.50	108.20
1	X	689	A	C1'-O4'-C4'	-6.62	104.60	109.90
1	X	1938	U	N1-C1'-C2'	6.62	122.60	114.00
1	X	2697	G	C2-N3-C4	6.62	115.21	111.90
1	X	989	G	O4'-C1'-N9	6.61	113.49	108.20
1	X	2735	C	O4'-C1'-N1	6.61	113.49	108.20
1	X	613	A	P-O3'-C3'	6.61	127.63	119.70
1	X	677	G	C4'-C3'-C2'	-6.61	95.99	102.60
1	X	725	C	O4'-C1'-N1	6.61	113.49	108.20
1	X	1288	A	C8-N9-C1'	-6.60	115.82	127.70
1	X	1469	U	N3-C2-O2	-6.60	117.58	122.20
1	X	1467	U	C4'-C3'-C2'	6.59	109.19	102.60
1	X	2181	A	C1'-O4'-C4'	-6.59	104.62	109.90
1	X	1120	C	P-O3'-C3'	6.59	127.61	119.70
1	X	2841	U	O4'-C1'-N1	6.59	113.47	108.20
1	X	2274	C	O4'-C1'-N1	6.59	113.47	108.20
1	X	2734	U	O4'-C1'-N1	6.59	113.47	108.20
1	X	1325	U	P-O3'-C3'	6.58	127.60	119.70
1	X	1292	A	O4'-C1'-N9	6.58	113.46	108.20
1	X	2383	C	O4'-C1'-N1	6.58	113.46	108.20
1	X	467	U	O4'-C4'-C3'	-6.57	97.43	104.00
1	X	651	C	O4'-C1'-N1	6.57	113.46	108.20
1	X	97	U	O4'-C1'-N1	6.57	113.45	108.20
1	X	1683	G	O4'-C1'-N9	6.57	113.45	108.20
1	X	2431	C	O4'-C1'-N1	6.56	113.45	108.20
1	X	617	U	O4'-C1'-N1	6.56	113.45	108.20
1	X	1696	C	O4'-C1'-N1	6.56	113.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	788	G	C2'-C3'-O3'	6.56	124.19	113.70
1	X	1549	C	O4'-C1'-N1	6.55	113.44	108.20
1	X	1882	G	C3'-C2'-C1'	6.55	106.74	101.50
1	X	1412	C	C2'-C3'-O3'	6.54	124.17	113.70
1	X	575	U	O4'-C1'-N1	6.54	113.43	108.20
1	X	2239	C	O4'-C1'-N1	6.54	113.43	108.20
1	X	2708	U	P-O3'-C3'	-6.54	111.86	119.70
1	X	2860	C	O4'-C1'-N1	6.53	113.43	108.20
1	X	1411	C	O4'-C1'-N1	6.53	113.42	108.20
1	X	819	C	O5'-P-OP2	-6.53	99.82	105.70
1	X	1909	U	C2-N1-C1'	6.53	125.53	117.70
1	X	1403	U	P-O3'-C3'	6.53	127.53	119.70
1	X	1989	C	C1'-O4'-C4'	6.53	115.12	109.90
1	X	2804	G	C5-C6-N1	6.52	114.76	111.50
1	X	738	G	N7-C8-N9	6.52	116.36	113.10
1	X	2628	C	C3'-C2'-C1'	-6.52	96.29	101.50
1	X	527	C	N1-C2-O2	6.51	122.81	118.90
1	X	955	G	N9-C1'-C2'	6.51	122.47	114.00
1	X	2553	G	C5-N7-C8	-6.51	101.05	104.30
1	X	2482	A	C5'-C4'-O4'	6.50	116.90	109.10
1	X	746	G	N3-C4-C5	-6.50	125.35	128.60
1	X	1032	A	C5-N7-C8	-6.50	100.65	103.90
1	X	1992	G	OP1-P-OP2	-6.50	109.86	119.60
1	X	2797	G	N3-C4-N9	6.50	129.90	126.00
2	Y	54	U	P-O5'-C5'	6.49	131.29	120.90
1	X	2691	C	O4'-C1'-N1	6.49	113.39	108.20
1	X	2553	G	C4-C5-N7	6.48	113.39	110.80
1	X	2656	G	O4'-C1'-N9	6.48	113.38	108.20
1	X	114	C	O4'-C1'-N1	6.48	113.38	108.20
1	X	243	G	P-O5'-C5'	6.47	131.25	120.90
1	X	540	G	C4'-C3'-C2'	-6.47	96.13	102.60
1	X	234	C	O4'-C1'-N1	6.47	113.38	108.20
1	X	467	U	C3'-C2'-C1'	-6.47	96.33	101.50
1	X	591	G	O4'-C1'-N9	6.47	113.38	108.20
1	X	1752	U	O4'-C1'-N1	6.47	113.38	108.20
1	X	2591	C	O4'-C1'-N1	6.47	113.38	108.20
1	X	549	G	O4'-C1'-N9	6.47	113.37	108.20
1	X	2437	G	O4'-C1'-N9	6.47	113.37	108.20
1	X	19	C	O4'-C1'-N1	6.46	113.37	108.20
1	X	569	C	P-O3'-C3'	-6.46	111.94	119.70
1	X	796	A	C6-C5-N7	-6.46	127.78	132.30
1	X	1663	C	P-O3'-C3'	6.46	127.45	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1223	G	C4-C5-N7	6.46	113.38	110.80
1	X	160	C	O4'-C1'-N1	6.46	113.37	108.20
1	X	648	A	P-O3'-C3'	6.46	127.45	119.70
1	X	483	A	C3'-C2'-C1'	-6.46	96.33	101.50
1	X	879	A	O4'-C1'-N9	-6.46	103.03	108.20
2	Y	70	C	O4'-C1'-N1	6.46	113.36	108.20
1	X	759	C	C5'-C4'-C3'	-6.45	105.68	116.00
1	X	1825	C	O4'-C1'-N1	6.45	113.36	108.20
1	X	649	G	O4'-C1'-N9	6.45	113.36	108.20
1	X	689	A	C8-N9-C4	-6.45	103.22	105.80
1	X	2815	C	O4'-C1'-N1	6.45	113.36	108.20
1	X	22	C	P-O3'-C3'	6.45	127.44	119.70
1	X	1811	A	C2'-C3'-O3'	6.45	124.01	113.70
1	X	1313	U	C1'-O4'-C4'	-6.44	104.75	109.90
1	X	1749	G	P-O3'-C3'	6.44	127.43	119.70
1	X	606	A	O4'-C4'-C3'	-6.43	97.57	104.00
1	X	1044	U	O4'-C1'-N1	6.43	113.34	108.20
1	X	2726	U	O4'-C1'-N1	6.43	113.34	108.20
1	X	1388	C	O4'-C1'-N1	6.43	113.34	108.20
1	X	1413	U	O4'-C1'-N1	6.43	113.34	108.20
1	X	2262	C	O4'-C1'-N1	6.43	113.34	108.20
1	X	2591	C	C5-C6-N1	6.43	124.21	121.00
1	X	496	C	P-O3'-C3'	-6.42	111.99	119.70
1	X	2019	C	O4'-C1'-N1	6.42	113.34	108.20
1	X	774	A	C4-C5-C6	6.42	120.21	117.00
1	X	2530	C	O5'-P-OP2	-6.42	99.92	105.70
1	X	2426	G	C5'-C4'-C3'	-6.42	105.74	116.00
1	X	784	U	O4'-C1'-N1	6.41	113.33	108.20
1	X	665	A	O4'-C1'-N9	6.41	113.33	108.20
1	X	1570	C	N1-C2-O2	6.41	122.74	118.90
1	X	2782	G	C6-C5-N7	-6.41	126.56	130.40
1	X	1249	G	C2'-C3'-O3'	6.41	123.95	113.70
1	X	1561	A	C4'-C3'-O3'	6.41	125.81	113.00
1	X	1943	A	C4'-C3'-C2'	6.40	109.00	102.60
1	X	1768	U	N1-C2-O2	6.40	127.28	122.80
1	X	2675	U	O4'-C1'-N1	6.40	113.32	108.20
1	X	71	A	C4'-C3'-C2'	6.40	109.00	102.60
1	X	758	G	P-O3'-C3'	6.39	127.37	119.70
1	X	2452	U	O4'-C1'-N1	6.39	113.32	108.20
1	X	774	A	C5'-C4'-O4'	6.39	116.77	109.10
1	X	890	U	O4'-C1'-N1	6.39	113.31	108.20
1	X	2256	G	C8-N9-C4	-6.38	103.85	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	173	A	O4'-C1'-N9	6.37	113.30	108.20
1	X	1489	C	O4'-C1'-N1	6.37	113.30	108.20
1	X	1770	U	C1'-O4'-C4'	-6.37	104.80	109.90
1	X	2782	G	C4-C5-N7	6.37	113.35	110.80
1	X	2439	U	O4'-C1'-N1	6.37	113.29	108.20
1	X	841	G	C1'-O4'-C4'	-6.37	104.81	109.90
1	X	738	G	C8-N9-C4	-6.36	103.86	106.40
1	X	220	U	O4'-C1'-N1	6.36	113.29	108.20
1	X	483	A	C4'-C3'-C2'	6.36	108.96	102.60
1	X	504	G	O4'-C4'-C3'	-6.36	97.64	104.00
1	X	542	A	C5-N7-C8	-6.36	100.72	103.90
1	X	1468	A	N3-C4-C5	-6.36	122.35	126.80
1	X	2291	U	O4'-C1'-N1	6.35	113.28	108.20
1	X	869	C	O4'-C1'-N1	6.34	113.27	108.20
1	X	1764	A	N1-C6-N6	6.34	122.40	118.60
1	X	522	G	O4'-C1'-N9	6.33	113.27	108.20
1	X	1122	A	O4'-C1'-N9	6.33	113.26	108.20
1	X	1334	A	C3'-C2'-C1'	-6.33	96.44	101.50
1	X	2678	C	O4'-C1'-N1	6.32	113.26	108.20
1	X	66	U	O4'-C1'-N1	6.32	113.26	108.20
1	X	539	A	O4'-C1'-N9	6.32	113.26	108.20
1	X	858	G	O4'-C1'-N9	6.32	113.26	108.20
1	X	501	G	O4'-C1'-N9	6.32	113.25	108.20
1	X	540	G	C2-N3-C4	6.32	115.06	111.90
1	X	1831	G	C8-N9-C4	-6.31	103.87	106.40
1	X	1144	U	O4'-C1'-N1	6.31	113.25	108.20
11	I	28	LYS	C-N-CA	6.31	137.47	121.70
1	X	2500	C	O4'-C1'-N1	6.31	113.25	108.20
1	X	2795	A	O4'-C1'-N9	-6.30	103.16	108.20
1	X	537	C	C2-N3-C4	-6.30	116.75	119.90
1	X	656	U	P-O5'-C5'	6.30	130.98	120.90
1	X	2189	A	N7-C8-N9	6.30	116.95	113.80
1	X	1407	G	N9-C1'-C2'	6.29	122.18	114.00
1	X	399	G	C2'-C3'-O3'	6.29	123.76	113.70
1	X	579	G	O4'-C1'-N9	6.29	113.23	108.20
1	X	1278	A	N9-C1'-C2'	6.29	122.17	114.00
1	X	432	C	O4'-C1'-N1	6.28	113.23	108.20
1	X	1997	A	P-O3'-C3'	6.28	127.24	119.70
1	X	1247	U	O4'-C1'-N1	6.28	113.22	108.20
1	X	2482	A	N1-C2-N3	-6.28	126.16	129.30
1	X	2540	A	O4'-C1'-N9	6.28	113.22	108.20
1	X	878	C	N1-C2-O2	6.28	122.67	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	467	U	N1-C1'-C2'	6.28	122.16	114.00
1	X	2318	U	O4'-C1'-N1	6.28	113.22	108.20
1	X	2074	U	O4'-C1'-N1	6.27	113.22	108.20
1	X	1314	A	N9-C1'-C2'	6.26	122.14	114.00
1	X	1963	G	N3-C4-C5	-6.26	125.47	128.60
1	X	657	A	C3'-C2'-C1'	-6.26	96.49	101.50
1	X	434	C	P-O3'-C3'	6.26	127.21	119.70
1	X	729	A	P-O3'-C3'	6.25	127.21	119.70
1	X	2639	A	P-O3'-C3'	-6.25	112.19	119.70
1	X	237	G	O4'-C1'-N9	6.25	113.20	108.20
1	X	413	G	N7-C8-N9	6.25	116.23	113.10
1	X	559	C	C2'-C3'-O3'	6.25	123.69	113.70
1	X	2393	G	O4'-C1'-N9	6.25	113.20	108.20
1	X	2705	A	C4'-C3'-C2'	6.25	108.85	102.60
1	X	332	C	O4'-C1'-N1	6.25	113.20	108.20
1	X	1990	U	N3-C2-O2	-6.25	117.83	122.20
1	X	1001	A	O4'-C1'-N9	6.24	113.19	108.20
1	X	1111	C	O4'-C1'-N1	6.24	113.19	108.20
1	X	879	A	C4'-C3'-C2'	6.24	108.84	102.60
1	X	1051	U	O4'-C1'-N1	6.24	113.19	108.20
1	X	187	U	O4'-C1'-N1	6.24	113.19	108.20
1	X	1598	C	O4'-C1'-N1	6.24	113.19	108.20
1	X	2081	U	O4'-C1'-N1	6.24	113.19	108.20
1	X	2594	U	C4-C5-C6	-6.24	115.96	119.70
1	X	2359	U	O4'-C1'-N1	6.23	113.19	108.20
1	X	780	U	C3'-C2'-C1'	-6.23	96.52	101.50
1	X	675	C	O4'-C1'-N1	6.22	113.18	108.20
1	X	2800	C	O4'-C1'-N1	6.22	113.18	108.20
1	X	1909	U	N1-C1'-C2'	6.22	122.08	114.00
1	X	1341	G	P-O3'-C3'	-6.21	112.25	119.70
1	X	2692	A	O5'-P-OP1	6.21	118.16	110.70
2	Y	83	C	N1-C2-O2	6.21	122.63	118.90
1	X	683	A	N9-C1'-C2'	6.21	122.07	114.00
1	X	1669	A	P-O5'-C5'	6.21	130.83	120.90
1	X	148	C	O4'-C1'-N1	6.21	113.17	108.20
1	X	1353	A	P-O3'-C3'	6.20	127.14	119.70
1	X	1373	G	O4'-C1'-N9	6.20	113.16	108.20
1	X	2181	A	O4'-C1'-N9	6.20	113.16	108.20
1	X	1991	C	P-O3'-C3'	-6.20	112.26	119.70
1	X	1624	A	C1'-O4'-C4'	-6.20	104.94	109.90
2	Y	45	C	N1-C2-O2	6.20	122.62	118.90
1	X	236	C	N1-C2-O2	6.19	122.62	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1621	C	O4'-C1'-N1	6.19	113.16	108.20
1	X	1288	A	N9-C1'-C2'	6.19	122.05	114.00
1	X	1819	U	O4'-C1'-N1	6.19	113.15	108.20
1	X	1882	G	P-O3'-C3'	6.19	127.13	119.70
1	X	2627	G	N1-C6-O6	6.19	123.61	119.90
1	X	595	A	O4'-C1'-N9	6.18	113.15	108.20
1	X	1953	A	C5'-C4'-O4'	6.18	116.52	109.10
1	X	956	A	C5-C6-N6	-6.18	118.75	123.70
1	X	346	C	C5-C6-N1	6.18	124.09	121.00
1	X	1075	C	O4'-C1'-N1	6.18	113.14	108.20
1	X	1288	A	C5'-C4'-C3'	6.18	125.89	116.00
1	X	857	U	O4'-C1'-N1	6.18	113.14	108.20
1	X	995	A	C3'-C2'-C1'	-6.18	96.56	101.50
1	X	1059	A	P-O3'-C3'	6.17	127.11	119.70
1	X	1467	U	N1-C1'-C2'	6.17	122.03	114.00
1	X	1983	G	P-O3'-C3'	6.17	127.11	119.70
1	X	2408	G	P-O3'-C3'	-6.17	112.30	119.70
1	X	2867	G	C6-C5-N7	-6.17	126.70	130.40
1	X	780	U	C2'-C3'-O3'	6.17	123.57	113.70
2	Y	87	C	O4'-C1'-N1	6.17	113.14	108.20
1	X	323	G	P-O5'-C5'	-6.17	111.03	120.90
1	X	2627	G	C5-C6-O6	-6.17	124.90	128.60
1	X	1505	U	O4'-C1'-N1	6.16	113.13	108.20
1	X	1579	G	O4'-C1'-N9	6.16	113.13	108.20
1	X	1006	C	P-O3'-C3'	6.16	127.09	119.70
1	X	169	C	N1-C2-O2	6.16	122.60	118.90
1	X	322	A	P-O3'-C3'	6.16	127.09	119.70
1	X	1338	G	C5-C6-O6	-6.16	124.90	128.60
1	X	1417	C	O4'-C1'-N1	6.16	113.13	108.20
1	X	1850	G	O4'-C1'-N9	6.16	113.13	108.20
1	X	1647	U	O4'-C1'-N1	6.16	113.12	108.20
1	X	393	U	O4'-C1'-N1	6.15	113.12	108.20
1	X	682	G	P-O3'-C3'	6.15	127.08	119.70
1	X	1398	G	O4'-C1'-N9	6.15	113.12	108.20
1	X	358	C	C6-N1-C2	-6.15	117.84	120.30
1	X	859	U	C5'-C4'-O4'	6.15	116.48	109.10
1	X	917	U	O4'-C1'-N1	6.15	113.12	108.20
1	X	1142	G	C1'-O4'-C4'	-6.14	104.98	109.90
1	X	796	A	C5-C6-N1	-6.14	114.63	117.70
1	X	1234	C	N1-C2-O2	6.14	122.58	118.90
1	X	542	A	C4-C5-C6	6.14	120.07	117.00
1	X	516	G	O4'-C1'-N9	6.14	113.11	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1981	A	O5'-P-OP2	-6.14	100.17	105.70
1	X	466	A	P-O3'-C3'	6.14	127.06	119.70
1	X	1032	A	N7-C8-N9	6.14	116.87	113.80
2	Y	32	C	C6-N1-C2	-6.14	117.84	120.30
1	X	193	A	O4'-C1'-N9	6.13	113.11	108.20
1	X	1467	U	C5-C4-O4	-6.13	122.22	125.90
2	Y	110	U	O4'-C1'-N1	6.13	113.11	108.20
1	X	2238	G	O4'-C1'-N9	6.13	113.11	108.20
1	X	2492	G	C8-N9-C4	-6.13	103.95	106.40
23	U	18	VAL	C-N-CA	6.13	137.03	121.70
1	X	387	A	C5'-C4'-O4'	6.13	116.45	109.10
1	X	982	C	O4'-C1'-N1	6.13	113.10	108.20
1	X	1496	G	C2'-C3'-O3'	6.13	123.50	113.70
1	X	2636	A	O4'-C1'-N9	6.13	113.10	108.20
1	X	321	A	P-O3'-C3'	6.12	127.05	119.70
1	X	1788	C	O4'-C1'-N1	6.12	113.10	108.20
1	X	1336	G	C5-C6-N1	6.12	114.56	111.50
1	X	244	C	O4'-C1'-N1	6.12	113.09	108.20
1	X	1468	A	N9-C1'-C2'	6.12	121.95	114.00
1	X	1792	C	P-O3'-C3'	6.12	127.04	119.70
1	X	2229	G	C8-N9-C4	-6.12	103.95	106.40
1	X	2809	A	P-O3'-C3'	6.12	127.04	119.70
1	X	2711	G	C5-C6-O6	-6.11	124.93	128.60
1	X	30	G	C8-N9-C4	-6.11	103.95	106.40
1	X	1017	C	O4'-C1'-N1	6.11	113.09	108.20
1	X	2312	A	O4'-C1'-N9	6.11	113.09	108.20
1	X	422	C	O4'-C1'-N1	6.11	113.08	108.20
1	X	29	U	O4'-C1'-N1	6.10	113.08	108.20
1	X	1380	C	O4'-C1'-N1	6.10	113.08	108.20
1	X	2844	G	O4'-C1'-N9	6.10	113.08	108.20
1	X	668	A	P-O3'-C3'	6.09	127.01	119.70
1	X	162	C	O4'-C1'-N1	6.09	113.07	108.20
19	Q	61	LYS	N-CA-C	6.09	127.45	111.00
1	X	707	U	O4'-C1'-N1	6.09	113.07	108.20
1	X	1181	C	O4'-C1'-N1	6.09	113.07	108.20
1	X	700	C	O4'-C1'-N1	6.09	113.07	108.20
1	X	1515	U	O4'-C1'-N1	6.09	113.07	108.20
9	G	103	TYR	C-N-CA	6.09	136.92	121.70
1	X	358	C	P-O5'-C5'	6.08	130.64	120.90
1	X	596	C	P-O5'-C5'	-6.08	111.17	120.90
1	X	2018	G	C1'-O4'-C4'	-6.08	105.03	109.90
1	X	396	U	C1'-O4'-C4'	-6.08	105.03	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	399	G	C4'-C3'-C2'	6.08	108.68	102.60
1	X	1540	C	O4'-C1'-N1	6.08	113.06	108.20
1	X	1142	G	O4'-C1'-C2'	-6.08	99.72	105.80
1	X	776	G	N9-C1'-C2'	6.08	121.90	114.00
1	X	1149	G	P-O3'-C3'	6.08	127.00	119.70
1	X	1233	A	C2'-C3'-O3'	6.08	123.43	113.70
1	X	1522	C	N1-C2-O2	6.08	122.55	118.90
1	X	135	U	O4'-C1'-N1	6.08	113.06	108.20
1	X	2554	C	N1-C2-O2	6.07	122.54	118.90
1	X	1466	C	O4'-C1'-N1	6.07	113.06	108.20
1	X	2414	A	P-O5'-C5'	6.07	130.61	120.90
1	X	618	A	O4'-C1'-N9	6.07	113.05	108.20
1	X	331	U	O4'-C1'-N1	6.06	113.05	108.20
1	X	113	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	1060	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	1758	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	2039	G	C5-C6-O6	-6.06	124.97	128.60
1	X	2184	C	O4'-C1'-N1	6.06	113.05	108.20
1	X	346	C	N3-C4-C5	-6.06	119.48	121.90
1	X	1006	C	N1-C1'-C2'	6.05	121.87	114.00
1	X	2336	G	O5'-P-OP2	-6.05	100.25	105.70
11	I	36	GLY	C-N-CA	6.05	136.83	121.70
1	X	1149	G	O4'-C1'-N9	6.05	113.04	108.20
1	X	1843	U	O4'-C1'-N1	6.05	113.04	108.20
1	X	1287	A	N1-C6-N6	-6.05	114.97	118.60
1	X	1353	A	O4'-C1'-N9	6.05	113.04	108.20
1	X	2661	G	O4'-C1'-N9	6.05	113.04	108.20
1	X	2685	A	C5-C6-N1	6.05	120.72	117.70
1	X	2281	C	O4'-C1'-N1	6.04	113.04	108.20
1	X	219	G	N9-C1'-C2'	6.04	121.85	114.00
1	X	90	G	N3-C4-C5	-6.04	125.58	128.60
1	X	473	C	OP2-P-O3'	6.04	118.48	105.20
1	X	1732	U	P-O3'-C3'	6.04	126.95	119.70
1	X	2295	C	O4'-C1'-N1	6.03	113.03	108.20
1	X	2799	C	C5-C4-N4	-6.03	115.98	120.20
1	X	1182	U	C2'-C3'-O3'	6.03	123.35	113.70
1	X	2264	C	O4'-C1'-N1	6.03	113.02	108.20
1	X	393	U	N3-C4-O4	6.03	123.62	119.40
1	X	833	A	N1-C6-N6	6.03	122.22	118.60
1	X	1333	G	C6-C5-N7	6.03	134.02	130.40
2	Y	54	U	C4'-C3'-C2'	-6.02	96.58	102.60
1	X	957	G	P-O3'-C3'	6.02	126.93	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2548	G	O4'-C4'-C3'	-6.02	97.98	104.00
1	X	1976	U	O4'-C1'-N1	6.02	113.01	108.20
1	X	2443	C	O4'-C1'-N1	6.01	113.01	108.20
1	X	2325	A	P-O3'-C3'	6.01	126.91	119.70
1	X	2558	C	O4'-C1'-N1	6.01	113.01	108.20
1	X	1655	C	O4'-C1'-N1	6.01	113.01	108.20
1	X	1913	G	P-O3'-C3'	6.01	126.91	119.70
1	X	2363	G	O4'-C1'-N9	6.01	113.01	108.20
1	X	724	C	O4'-C1'-N1	6.00	113.00	108.20
1	X	1324	G	O4'-C1'-N9	6.00	113.00	108.20
1	X	577	U	O4'-C1'-N1	6.00	113.00	108.20
1	X	2608	A	C1'-O4'-C4'	-6.00	105.10	109.90
2	Y	50	U	O4'-C1'-N1	6.00	113.00	108.20
1	X	1548	U	O4'-C1'-N1	5.99	112.99	108.20
2	Y	7	C	O4'-C1'-N1	5.99	112.99	108.20
1	X	413	G	N3-C4-C5	-5.99	125.61	128.60
1	X	1946	U	C2-N1-C1'	5.99	124.89	117.70
1	X	1099	A	P-O3'-C3'	5.99	126.88	119.70
1	X	338	G	C8-N9-C4	-5.99	104.01	106.40
1	X	1541	G	C4'-C3'-C2'	-5.99	96.61	102.60
1	X	2408	G	OP1-P-OP2	-5.99	110.62	119.60
1	X	2645	C	N1-C2-O2	5.99	122.49	118.90
11	I	41	SER	N-CA-C	5.99	127.16	111.00
1	X	221	A	O4'-C1'-N9	5.98	112.99	108.20
1	X	1573	G	P-O3'-C3'	5.98	126.88	119.70
1	X	302	U	O4'-C1'-N1	5.98	112.98	108.20
1	X	1461	C	O4'-C1'-N1	5.98	112.98	108.20
1	X	2371	A	C8-N9-C4	-5.98	103.41	105.80
1	X	779	U	O4'-C1'-N1	5.97	112.98	108.20
1	X	2193	C	O4'-C4'-C3'	-5.97	98.03	104.00
11	I	38	LYS	C-N-CA	5.97	136.63	121.70
1	X	223	C	O4'-C1'-N1	5.97	112.98	108.20
1	X	714	G	C3'-C2'-C1'	-5.97	96.72	101.50
1	X	2194	A	P-O3'-C3'	5.97	126.86	119.70
1	X	2775	U	O4'-C1'-N1	5.97	112.97	108.20
1	X	946	U	O4'-C1'-N1	5.97	112.97	108.20
1	X	1345	G	O5'-P-OP2	-5.97	100.33	105.70
1	X	2482	A	C2-N3-C4	5.97	113.58	110.60
1	X	2561	G	C4-C5-N7	5.96	113.19	110.80
1	X	1002	C	C6-N1-C2	-5.96	117.92	120.30
1	X	822	G	C4'-C3'-C2'	-5.96	96.64	102.60
1	X	1142	G	C3'-C2'-C1'	-5.96	96.73	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1030	U	O4'-C1'-N1	5.96	112.97	108.20
1	X	2719	U	O4'-C1'-N1	5.96	112.97	108.20
1	X	559	C	P-O3'-C3'	5.96	126.85	119.70
1	X	1950	C	O4'-C1'-N1	5.96	112.97	108.20
1	X	2683	C	O4'-C1'-N1	5.96	112.96	108.20
1	X	2408	G	N3-C4-C5	-5.95	125.62	128.60
1	X	2324	G	P-O3'-C3'	5.94	126.83	119.70
1	X	224	G	C5'-C4'-O4'	5.94	116.23	109.10
1	X	2258	G	C4'-C3'-C2'	-5.94	96.66	102.60
1	X	2858	A	O4'-C1'-N9	5.94	112.95	108.20
1	X	1336	G	C4-C5-N7	5.94	113.17	110.80
1	X	1530	U	O4'-C1'-N1	5.94	112.95	108.20
1	X	656	U	C1'-O4'-C4'	-5.94	105.15	109.90
1	X	2681	A	C5-C6-N1	5.94	120.67	117.70
15	M	28	ARG	N-CA-C	-5.93	94.98	111.00
1	X	1338	G	N3-C4-C5	-5.93	125.64	128.60
1	X	1350	G	C5-C6-O6	-5.93	125.04	128.60
2	Y	58	G	C3'-C2'-C1'	5.93	106.24	101.50
1	X	979	A	O4'-C1'-N9	5.93	112.94	108.20
1	X	2478	C	C6-N1-C2	-5.93	117.93	120.30
1	X	2552	C	C4'-C3'-C2'	-5.93	96.67	102.60
1	X	2576	G	O4'-C1'-N9	-5.93	103.46	108.20
1	X	1311	C	O4'-C1'-N1	5.92	112.94	108.20
2	Y	24	U	O4'-C1'-N1	5.92	112.94	108.20
1	X	2699	G	P-O3'-C3'	5.92	126.81	119.70
1	X	520	C	C4'-C3'-C2'	-5.92	96.68	102.60
1	X	2257	A	P-O5'-C5'	5.92	130.37	120.90
1	X	68	C	N1-C2-O2	5.92	122.45	118.90
1	X	2354	G	O4'-C4'-C3'	-5.92	98.08	104.00
1	X	242	A	P-O5'-C5'	5.92	130.36	120.90
1	X	567	G	O4'-C1'-N9	5.91	112.93	108.20
1	X	1468	A	C6-N1-C2	-5.91	115.05	118.60
1	X	1805	G	O4'-C1'-N9	5.91	112.93	108.20
1	X	841	G	C5-N7-C8	-5.91	101.35	104.30
1	X	1754	G	P-O5'-C5'	5.91	130.35	120.90
1	X	2406	C	P-O5'-C5'	5.91	130.35	120.90
1	X	2690	A	O4'-C1'-N9	5.91	112.93	108.20
1	X	865	A	O4'-C1'-N9	5.91	112.93	108.20
1	X	2382	C	C6-N1-C2	-5.91	117.94	120.30
1	X	825	C	P-O5'-C5'	5.91	130.35	120.90
1	X	1304	U	O4'-C1'-N1	5.91	112.92	108.20
1	X	1412	C	O4'-C4'-C3'	-5.91	98.09	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1667	A	O4'-C1'-N9	5.90	112.92	108.20
1	X	2578	G	P-O5'-C5'	5.90	130.35	120.90
1	X	2267	A	P-O3'-C3'	5.90	126.78	119.70
1	X	2854	G	O4'-C1'-C2'	-5.90	99.90	105.80
1	X	2045	A	C3'-C2'-C1'	5.90	106.22	101.50
1	X	2560	G	N3-C4-C5	-5.90	125.65	128.60
1	X	2593	A	P-O3'-C3'	5.90	126.78	119.70
1	X	1064	C	O4'-C1'-N1	5.90	112.92	108.20
1	X	154	U	O4'-C1'-N1	5.90	112.92	108.20
1	X	811	G	N1-C6-O6	-5.90	116.36	119.90
1	X	1454	U	N3-C4-O4	5.90	123.53	119.40
1	X	622	U	O4'-C1'-N1	5.89	112.91	108.20
1	X	2847	G	C8-N9-C4	-5.89	104.04	106.40
1	X	338	G	O4'-C1'-N9	5.89	112.91	108.20
1	X	1313	U	O4'-C1'-N1	5.89	112.91	108.20
1	X	2560	G	C5-C6-O6	-5.89	125.07	128.60
2	Y	22	U	O4'-C1'-N1	5.89	112.91	108.20
1	X	2692	A	P-O3'-C3'	5.88	126.76	119.70
1	X	466	A	P-O5'-C5'	5.88	130.31	120.90
1	X	681	A	C8-N9-C4	-5.88	103.45	105.80
1	X	2366	U	O4'-C1'-N1	5.88	112.91	108.20
1	X	2484	G	C8-N9-C4	-5.88	104.05	106.40
1	X	983	G	P-O3'-C3'	5.88	126.75	119.70
1	X	430	C	C5-C6-N1	5.88	123.94	121.00
1	X	1265	G	O5'-P-OP2	-5.87	100.42	105.70
1	X	955	G	N3-C4-C5	-5.87	125.67	128.60
1	X	1090	C	O4'-C1'-N1	5.87	112.89	108.20
1	X	2229	G	C5'-C4'-O4'	5.87	116.14	109.10
1	X	320	A	C2-N3-C4	5.87	113.53	110.60
1	X	431	G	O4'-C1'-N9	5.87	112.89	108.20
1	X	1338	G	N3-C4-N9	5.87	129.52	126.00
1	X	1468	A	C2-N3-C4	5.86	113.53	110.60
1	X	2018	G	N7-C8-N9	5.86	116.03	113.10
1	X	791	G	P-O3'-C3'	5.86	126.73	119.70
1	X	1922	U	N3-C2-O2	-5.86	118.10	122.20
1	X	2826	C	C4'-C3'-C2'	-5.86	96.75	102.60
1	X	2587	G	O4'-C1'-N9	5.85	112.88	108.20
1	X	1775	A	C4'-C3'-O3'	-5.85	97.11	109.40
1	X	2875	C	O4'-C1'-N1	5.85	112.88	108.20
1	X	679	C	O4'-C1'-N1	5.84	112.87	108.20
1	X	2478	C	P-O3'-C3'	-5.84	112.69	119.70
2	Y	81	C	C5-C6-N1	5.84	123.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2258	G	O4'-C1'-N9	5.84	112.87	108.20
1	X	309	G	N7-C8-N9	5.84	116.02	113.10
1	X	515	A	O4'-C1'-N9	5.84	112.87	108.20
1	X	651	C	P-O3'-C3'	5.83	126.70	119.70
1	X	731	A	O4'-C1'-N9	5.83	112.87	108.20
1	X	1087	C	P-O5'-C5'	5.83	130.23	120.90
1	X	2025	A	O4'-C1'-N9	5.83	112.86	108.20
1	X	1472	C	O4'-C1'-N1	5.83	112.86	108.20
1	X	1514	C	O4'-C1'-N1	5.83	112.86	108.20
1	X	1243	G	O4'-C1'-N9	5.82	112.86	108.20
1	X	2422	C	O4'-C1'-N1	5.82	112.86	108.20
1	X	1288	A	N9-C4-C5	-5.82	103.47	105.80
1	X	1695	U	C5'-C4'-O4'	5.82	116.08	109.10
1	X	1703	C	C3'-C2'-C1'	-5.82	96.85	101.50
1	X	1115	C	O4'-C1'-N1	5.81	112.85	108.20
1	X	757	U	OP2-P-O3'	5.81	117.98	105.20
2	Y	67	C	P-O3'-C3'	5.81	126.67	119.70
1	X	424	G	P-O3'-C3'	5.81	126.67	119.70
1	X	2806	G	O4'-C1'-N9	5.81	112.85	108.20
1	X	1367	A	O4'-C1'-N9	5.81	112.84	108.20
1	X	1328	C	O4'-C1'-N1	5.80	112.84	108.20
1	X	1407	G	P-O3'-C3'	5.80	126.67	119.70
1	X	1344	C	N3-C4-C5	5.80	124.22	121.90
1	X	1244	U	O4'-C1'-N1	5.80	112.84	108.20
1	X	2303	C	N1-C2-O2	5.80	122.38	118.90
1	X	747	A	P-O3'-C3'	-5.80	112.74	119.70
1	X	2321	C	C6-N1-C2	-5.80	117.98	120.30
1	X	1781	C	C5'-C4'-O4'	5.79	116.06	109.10
1	X	1288	A	N1-C6-N6	5.79	122.07	118.60
1	X	1506	C	O4'-C1'-N1	5.79	112.83	108.20
1	X	1831	G	N7-C8-N9	5.79	116.00	113.10
1	X	2075	U	C1'-O4'-C4'	-5.79	105.27	109.90
1	X	2485	U	C2-N1-C1'	5.79	124.65	117.70
1	X	1286	U	P-O5'-C5'	5.78	130.15	120.90
1	X	1680	U	C2'-C3'-O3'	5.78	122.95	113.70
1	X	2315	A	P-O5'-C5'	5.78	130.15	120.90
1	X	437	G	O4'-C1'-N9	5.78	112.82	108.20
1	X	1469	U	C5'-C4'-O4'	5.78	116.04	109.10
1	X	2006	G	O5'-P-OP1	-5.78	100.50	105.70
1	X	2541	U	N3-C2-O2	-5.78	118.15	122.20
1	X	559	C	N1-C2-O2	5.78	122.37	118.90
1	X	2406	C	O4'-C1'-N1	5.78	112.82	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	952	A	P-O5'-C5'	5.78	130.15	120.90
1	X	1097	A	P-O3'-C3'	5.78	126.63	119.70
1	X	2616	U	O4'-C1'-N1	5.78	112.82	108.20
1	X	2619	G	N7-C8-N9	5.78	115.99	113.10
1	X	1546	C	O4'-C1'-N1	5.78	112.82	108.20
1	X	873	U	O4'-C1'-N1	5.77	112.82	108.20
1	X	648	A	C1'-O4'-C4'	-5.77	105.28	109.90
1	X	683	A	C2'-C3'-O3'	5.77	122.94	113.70
1	X	1086	C	C3'-C2'-C1'	5.77	106.12	101.50
1	X	327	C	O4'-C1'-N1	5.77	112.81	108.20
1	X	508	G	O4'-C1'-N9	5.77	112.82	108.20
1	X	1092	U	O4'-C1'-N1	5.77	112.82	108.20
1	X	2795	A	C3'-C2'-C1'	5.77	106.11	101.50
1	X	2697	G	P-O3'-C3'	-5.77	112.78	119.70
1	X	2371	A	N7-C8-N9	5.76	116.68	113.80
1	X	1191	G	P-O3'-C3'	5.76	126.61	119.70
1	X	199	A	P-O3'-C3'	5.75	126.61	119.70
1	X	2668	U	N3-C4-O4	-5.75	115.37	119.40
14	L	88	VAL	C-N-CA	5.75	136.08	121.70
1	X	1363	C	O4'-C1'-N1	5.75	112.80	108.20
1	X	1806	G	C8-N9-C4	-5.75	104.10	106.40
1	X	2370	G	O4'-C1'-N9	5.75	112.80	108.20
1	X	1964	A	O4'-C1'-N9	5.75	112.80	108.20
1	X	3	U	O4'-C4'-C3'	-5.74	98.26	104.00
1	X	1010	U	N3-C2-O2	-5.74	118.18	122.20
1	X	1145	C	P-O3'-C3'	5.74	126.59	119.70
1	X	1712	G	C6-C5-N7	-5.74	126.95	130.40
1	X	2587	G	C5-C6-O6	-5.74	125.15	128.60
1	X	2869	U	O4'-C1'-N1	5.74	112.79	108.20
1	X	2256	G	O4'-C1'-N9	5.74	112.79	108.20
1	X	1265	G	P-O3'-C3'	5.74	126.58	119.70
1	X	1762	C	O4'-C1'-N1	5.74	112.79	108.20
1	X	2811	G	O4'-C1'-N9	5.74	112.79	108.20
1	X	1561	A	O4'-C4'-C3'	-5.73	98.27	104.00
1	X	339	U	P-O3'-C3'	5.73	126.58	119.70
9	G	108	GLY	N-CA-C	-5.73	98.78	113.10
1	X	322	A	O4'-C1'-N9	5.73	112.78	108.20
1	X	2329	C	O4'-C1'-N1	5.73	112.78	108.20
1	X	467	U	C5-C4-O4	-5.73	122.46	125.90
1	X	767	G	O4'-C1'-N9	5.72	112.78	108.20
1	X	955	G	N3-C4-N9	5.72	129.43	126.00
1	X	1575	C	C4'-C3'-C2'	5.72	108.32	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1467	U	C5'-C4'-O4'	-5.71	102.24	109.10
1	X	480	G	C5-C6-N1	5.71	114.36	111.50
1	X	537	C	N3-C4-C5	5.71	124.19	121.90
1	X	2230	G	C5-C6-O6	-5.71	125.17	128.60
1	X	2535	C	C5'-C4'-C3'	-5.71	106.86	116.00
1	X	777	A	C4'-C3'-C2'	5.71	108.31	102.60
1	X	2694	G	C5'-C4'-O4'	-5.71	102.25	109.10
1	X	2086	U	O4'-C1'-N1	5.70	112.76	108.20
1	X	2668	U	C5-C6-N1	-5.70	119.85	122.70
1	X	322	A	N9-C1'-C2'	5.70	121.41	114.00
1	X	1662	G	N9-C1'-C2'	5.70	121.41	114.00
1	X	660	G	C3'-C2'-C1'	-5.70	96.94	101.50
1	X	519	C	C5'-C4'-O4'	-5.70	102.26	109.10
1	X	1795	C	O4'-C1'-N1	5.70	112.76	108.20
2	Y	32	C	C5-C6-N1	5.70	123.85	121.00
1	X	1141	U	P-O3'-C3'	5.69	126.53	119.70
1	X	1631	C	N1-C1'-C2'	5.69	121.40	114.00
1	X	1828	C	O4'-C1'-N1	5.69	112.75	108.20
2	Y	111	C	P-O3'-C3'	5.69	126.53	119.70
2	Y	50	U	C3'-C2'-C1'	-5.69	96.95	101.50
1	X	1253	C	P-O3'-C3'	-5.69	112.88	119.70
1	X	1831	G	O4'-C1'-N9	5.69	112.75	108.20
1	X	1091	C	O4'-C1'-N1	5.69	112.75	108.20
1	X	1281	A	P-O3'-C3'	5.68	126.52	119.70
1	X	2495	G	O4'-C1'-N9	5.68	112.75	108.20
1	X	889	C	O4'-C1'-N1	5.68	112.75	108.20
1	X	955	G	N1-C2-N2	-5.68	111.09	116.20
1	X	1531	C	C1'-O4'-C4'	-5.68	105.36	109.90
1	X	2463	G	C5'-C4'-O4'	5.68	115.92	109.10
1	X	2552	C	N1-C1'-C2'	5.68	121.38	114.00
1	X	1063	C	O4'-C1'-N1	5.67	112.74	108.20
1	X	1182	U	O4'-C1'-N1	5.67	112.74	108.20
1	X	1105	U	O4'-C1'-N1	5.67	112.73	108.20
1	X	2528	G	OP1-P-O3'	5.67	117.67	105.20
1	X	1663	C	N3-C2-O2	-5.67	117.93	121.90
1	X	1824	C	C3'-C2'-C1'	-5.67	96.97	101.50
1	X	2080	U	O4'-C1'-N1	5.67	112.73	108.20
1	X	827	C	O4'-C1'-N1	5.67	112.73	108.20
1	X	2591	C	N1-C2-O2	5.67	122.30	118.90
1	X	2444	C	O4'-C1'-N1	5.66	112.73	108.20
1	X	816	U	O4'-C1'-N1	5.66	112.73	108.20
1	X	1076	U	O4'-C1'-N1	5.66	112.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2198	U	P-O3'-C3'	5.66	126.49	119.70
1	X	224	G	O4'-C1'-N9	5.66	112.72	108.20
1	X	975	C	O4'-C1'-N1	5.65	112.72	108.20
1	X	1531	C	O4'-C1'-N1	5.65	112.72	108.20
1	X	660	G	N3-C2-N2	-5.65	115.94	119.90
1	X	450	C	O4'-C1'-N1	5.65	112.72	108.20
1	X	545	C	C3'-C2'-C1'	-5.65	96.98	101.50
1	X	2745	A	C2-N3-C4	5.65	113.42	110.60
1	X	483	A	C5'-C4'-O4'	5.65	115.88	109.10
1	X	675	C	C3'-C2'-C1'	-5.65	96.98	101.50
1	X	1820	G	C4'-C3'-C2'	5.65	108.25	102.60
1	X	1347	C	OP2-P-O3'	5.65	117.62	105.20
2	Y	34	C	O4'-C1'-N1	5.65	112.72	108.20
2	Y	75	A	P-O3'-C3'	5.64	126.47	119.70
1	X	534	U	O4'-C1'-N1	5.64	112.71	108.20
1	X	702	A	O3'-P-O5'	-5.64	93.29	104.00
1	X	2485	U	N3-C2-O2	-5.64	118.25	122.20
1	X	332	C	P-O3'-C3'	5.64	126.47	119.70
1	X	1487	C	O4'-C1'-N1	5.63	112.71	108.20
1	X	540	G	C8-N9-C1'	-5.63	119.68	127.00
1	X	858	G	C3'-C2'-C1'	5.63	106.00	101.50
1	X	2481	G	O3'-P-O5'	-5.63	93.30	104.00
1	X	750	C	O4'-C1'-N1	5.63	112.70	108.20
1	X	1415	C	O4'-C1'-N1	5.63	112.70	108.20
1	X	219	G	O4'-C1'-C2'	-5.62	100.17	105.80
1	X	455	A	P-O3'-C3'	5.62	126.45	119.70
1	X	2479	U	C4'-C3'-C2'	-5.62	96.98	102.60
1	X	1241	G	O4'-C1'-N9	5.62	112.69	108.20
1	X	1567	A	O4'-C1'-N9	5.62	112.69	108.20
1	X	33	C	C4'-C3'-C2'	5.62	108.22	102.60
1	X	648	A	N9-C1'-C2'	5.62	121.30	114.00
1	X	2609	G	N3-C4-C5	-5.61	125.79	128.60
1	X	2417	U	P-O3'-C3'	5.61	126.44	119.70
1	X	1277	G	N3-C4-C5	-5.61	125.80	128.60
1	X	1266	G	N9-C1'-C2'	5.61	121.29	114.00
1	X	1925	C	O4'-C1'-N1	5.61	112.69	108.20
1	X	1833	U	O4'-C1'-N1	5.61	112.69	108.20
1	X	553	C	N1-C2-O2	5.61	122.26	118.90
1	X	827	C	P-O5'-C5'	5.61	129.87	120.90
1	X	879	A	C5'-C4'-C3'	-5.61	107.03	116.00
1	X	1249	G	N1-C6-O6	-5.61	116.54	119.90
1	X	1689	U	P-O3'-C3'	5.61	126.43	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1983	G	C4'-C3'-C2'	-5.61	97.00	102.60
1	X	2398	U	O4'-C1'-N1	5.60	112.68	108.20
1	X	1341	G	P-O5'-C5'	5.60	129.86	120.90
1	X	1547	U	O4'-C1'-N1	5.60	112.68	108.20
1	X	1570	C	C2-N1-C1'	5.60	124.96	118.80
1	X	2049	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	623	G	O4'-C1'-N9	5.60	112.68	108.20
1	X	208	C	O4'-C1'-N1	5.60	112.68	108.20
1	X	699	G	C8-N9-C4	-5.60	104.16	106.40
1	X	1298	G	OP2-P-O3'	5.60	117.52	105.20
1	X	1734	C	N1-C2-O2	5.60	122.26	118.90
1	X	995	A	N9-C1'-C2'	5.60	121.28	114.00
1	X	1031	C	N1-C2-O2	5.59	122.26	118.90
1	X	2237	C	P-O3'-C3'	5.59	126.41	119.70
1	X	36	G	C8-N9-C4	-5.59	104.16	106.40
1	X	1344	C	O4'-C4'-C3'	-5.59	98.41	104.00
1	X	1882	G	P-O5'-C5'	5.59	129.85	120.90
1	X	558	G	O4'-C1'-N9	5.59	112.67	108.20
12	J	88	LYS	C-N-CA	5.59	134.04	122.30
1	X	1224	A	P-O3'-C3'	5.59	126.40	119.70
1	X	1971	C	O4'-C1'-N1	5.59	112.67	108.20
1	X	81	C	O4'-C1'-N1	5.58	112.67	108.20
1	X	1570	C	C3'-C2'-C1'	-5.58	97.03	101.50
1	X	2018	G	C4-C5-C6	-5.58	115.45	118.80
1	X	1993	G	O4'-C1'-N9	5.58	112.67	108.20
1	X	2528	G	C8-N9-C4	-5.58	104.17	106.40
1	X	215	G	O4'-C1'-N9	5.58	112.66	108.20
1	X	1776	A	C2-N3-C4	5.58	113.39	110.60
1	X	2273	C	O4'-C1'-N1	5.58	112.66	108.20
1	X	2046	C	O4'-C1'-N1	5.58	112.66	108.20
1	X	753	U	C5'-C4'-O4'	-5.58	102.41	109.10
1	X	1333	G	C5-N7-C8	-5.57	101.51	104.30
1	X	2447	G	P-O3'-C3'	5.57	126.38	119.70
1	X	2675	U	N3-C2-O2	-5.57	118.30	122.20
1	X	337	G	C8-N9-C4	-5.57	104.17	106.40
1	X	820	U	P-O3'-C3'	-5.57	113.02	119.70
1	X	978	U	O4'-C1'-N1	5.57	112.65	108.20
1	X	607	C	O4'-C4'-C3'	-5.56	98.44	104.00
1	X	681	A	N7-C8-N9	5.56	116.58	113.80
1	X	479	G	C5-C6-O6	-5.56	125.27	128.60
1	X	770	U	C5-C4-O4	-5.56	122.56	125.90
1	X	1013	G	C8-N9-C4	-5.56	104.18	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1031	C	C4'-C3'-C2'	5.56	108.16	102.60
1	X	175	C	C6-N1-C2	-5.56	118.08	120.30
1	X	2314	A	P-O3'-C3'	5.56	126.37	119.70
1	X	838	A	C2-N3-C4	5.56	113.38	110.60
1	X	1033	G	C2'-C3'-O3'	5.56	122.59	113.70
1	X	1333	G	C4-C5-C6	-5.55	115.47	118.80
1	X	1	G	P-O3'-C3'	5.55	126.36	119.70
1	X	828	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	840	U	O5'-P-OP2	-5.55	100.70	105.70
1	X	418	C	C5'-C4'-C3'	5.55	124.88	116.00
1	X	876	A	O4'-C1'-N9	5.55	112.64	108.20
1	X	2504	G	O4'-C1'-N9	5.55	112.64	108.20
2	Y	72	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	359	G	O4'-C1'-N9	5.55	112.64	108.20
1	X	449	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	1623	C	N1-C2-O2	5.55	122.23	118.90
1	X	2759	U	P-O3'-C3'	5.55	126.36	119.70
1	X	647	G	P-O3'-C3'	5.54	126.35	119.70
1	X	1544	A	P-O3'-C3'	5.54	126.35	119.70
1	X	1700	C	P-O3'-C3'	-5.54	113.05	119.70
1	X	2575	U	C5-C4-O4	-5.54	122.57	125.90
1	X	2742	G	O4'-C1'-N9	5.54	112.64	108.20
1	X	2229	G	P-O5'-C5'	-5.54	112.03	120.90
19	Q	62	ARG	C-N-CA	5.54	135.55	121.70
1	X	1143	A	C1'-O4'-C4'	-5.54	105.47	109.90
1	X	1814	G	O4'-C1'-N9	5.54	112.63	108.20
1	X	1108	U	O4'-C1'-N1	5.54	112.63	108.20
1	X	1389	C	O4'-C1'-N1	5.54	112.63	108.20
1	X	1570	C	C6-N1-C1'	-5.54	114.16	120.80
1	X	168	A	O4'-C1'-N9	5.54	112.63	108.20
1	X	462	G	C4-C5-C6	5.54	122.12	118.80
1	X	985	G	C5-N7-C8	-5.53	101.53	104.30
1	X	1201	G	N3-C2-N2	-5.53	116.03	119.90
1	X	2591	C	C2-N3-C4	5.53	122.67	119.90
1	X	1016	C	O4'-C1'-N1	5.53	112.63	108.20
1	X	1469	U	O3'-P-O5'	5.53	114.51	104.00
1	X	99	U	C2-N1-C1'	5.53	124.34	117.70
1	X	211	U	O4'-C1'-N1	5.53	112.62	108.20
1	X	467	U	N3-C4-O4	5.53	123.27	119.40
1	X	1252	C	O4'-C1'-N1	5.53	112.62	108.20
1	X	972	C	C1'-O4'-C4'	-5.53	105.48	109.90
2	Y	6	C	O4'-C1'-N1	5.53	112.62	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2490	U	O4'-C1'-N1	5.53	112.62	108.20
1	X	990	A	O4'-C4'-C3'	-5.53	98.47	104.00
1	X	1963	G	C3'-C2'-C1'	5.53	105.92	101.50
1	X	2870	C	O4'-C1'-N1	5.52	112.62	108.20
1	X	22	C	O4'-C1'-N1	5.52	112.62	108.20
1	X	689	A	N1-C6-N6	5.52	121.91	118.60
1	X	796	A	C8-N9-C4	-5.52	103.59	105.80
1	X	823	U	C2'-C3'-O3'	5.52	122.53	113.70
1	X	2708	U	C5'-C4'-C3'	-5.52	107.16	116.00
17	O	97	GLY	N-CA-C	5.52	126.90	113.10
1	X	1699	A	C5-C6-N1	-5.52	114.94	117.70
1	X	2771	C	O4'-C1'-N1	5.52	112.61	108.20
1	X	447	U	P-O3'-C3'	5.52	126.32	119.70
1	X	1630	A	O3'-P-O5'	-5.52	93.52	104.00
1	X	2797	G	C6-C5-N7	-5.52	127.09	130.40
1	X	998	C	O4'-C1'-N1	5.51	112.61	108.20
1	X	2190	A	C5'-C4'-C3'	5.51	124.82	116.00
1	X	2199	C	N1-C1'-C2'	5.51	121.17	114.00
1	X	2560	G	C6-N1-C2	-5.51	121.79	125.10
1	X	652	C	P-O5'-C5'	-5.51	112.08	120.90
1	X	155	G	O4'-C1'-N9	5.51	112.61	108.20
1	X	448	C	N1-C2-O2	5.51	122.21	118.90
2	Y	19	C	N1-C2-O2	5.51	122.20	118.90
1	X	580	A	N9-C1'-C2'	5.51	121.16	114.00
1	X	2285	U	O4'-C1'-N1	5.51	112.61	108.20
1	X	2646	C	C6-N1-C2	-5.51	118.10	120.30
1	X	186	C	N1-C2-O2	5.51	122.20	118.90
1	X	555	U	P-O3'-C3'	5.51	126.31	119.70
1	X	1089	C	P-O3'-C3'	5.51	126.31	119.70
1	X	2255	G	C5-C6-O6	-5.51	125.30	128.60
2	Y	9	G	C3'-C2'-C1'	-5.50	97.10	101.50
1	X	309	G	C8-N9-C4	-5.50	104.20	106.40
1	X	1250	A	C5'-C4'-O4'	5.50	115.70	109.10
1	X	1337	G	O4'-C1'-N9	5.50	112.60	108.20
1	X	1442	C	C4'-C3'-C2'	5.50	108.10	102.60
1	X	303	C	O4'-C1'-N1	5.50	112.60	108.20
1	X	1280	U	C5-C6-N1	5.50	125.45	122.70
1	X	2772	U	O4'-C1'-N1	5.50	112.60	108.20
1	X	942	U	N3-C2-O2	-5.50	118.35	122.20
2	Y	30	C	P-O5'-C5'	5.50	129.70	120.90
1	X	63	A	C2-N3-C4	5.50	113.35	110.60
1	X	2619	G	C5-N7-C8	-5.49	101.55	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	7	G	C5'-C4'-C3'	-5.49	107.22	116.00
1	X	2018	G	C8-N9-C4	-5.49	104.20	106.40
2	Y	79	U	O4'-C1'-N1	5.49	112.59	108.20
1	X	180	C	O4'-C1'-N1	5.49	112.59	108.20
1	X	1169	C	O4'-C1'-N1	5.49	112.59	108.20
1	X	1513	U	O4'-C1'-N1	5.49	112.59	108.20
1	X	2222	U	N3-C2-O2	-5.49	118.36	122.20
1	X	2485	U	N1-C2-O2	5.48	126.64	122.80
1	X	2769	C	C5'-C4'-C3'	-5.48	107.23	116.00
2	Y	31	A	O4'-C1'-N9	5.48	112.59	108.20
19	Q	60	GLY	N-CA-C	5.48	126.80	113.10
1	X	2540	A	O4'-C4'-C3'	-5.48	98.52	104.00
1	X	1422	C	O4'-C1'-N1	5.48	112.58	108.20
1	X	1629	G	C4'-C3'-C2'	-5.48	97.12	102.60
1	X	2808	U	P-O5'-C5'	5.48	129.66	120.90
1	X	2867	G	C8-N9-C4	-5.48	104.21	106.40
1	X	1979	C	P-O3'-C3'	5.48	126.27	119.70
1	X	669	G	O4'-C4'-C3'	-5.47	98.53	104.00
1	X	2484	G	C2-N3-C4	5.47	114.64	111.90
1	X	103	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	1009	C	N1-C2-O2	5.47	122.18	118.90
1	X	1055	A	O4'-C1'-N9	5.47	112.58	108.20
1	X	1410	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	1977	C	O4'-C1'-N1	5.47	112.58	108.20
1	X	2409	A	N9-C1'-C2'	5.47	121.11	114.00
1	X	753	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	1939	U	O4'-C1'-N1	5.47	112.58	108.20
1	X	2533	U	C5-C6-N1	5.47	125.43	122.70
1	X	344	G	N9-C1'-C2'	5.46	121.10	114.00
1	X	761	G	P-O5'-C5'	-5.46	112.16	120.90
1	X	1713	G	P-O5'-C5'	5.46	129.64	120.90
1	X	126	C	O4'-C1'-N1	5.46	112.57	108.20
1	X	2782	G	C3'-C2'-C1'	-5.46	97.13	101.50
1	X	1745	C	C6-N1-C2	-5.46	118.12	120.30
1	X	542	A	C1'-O4'-C4'	5.46	114.27	109.90
1	X	1132	C	O4'-C1'-N1	5.46	112.57	108.20
1	X	112	U	N1-C1'-C2'	5.46	121.09	114.00
1	X	1870	U	O4'-C1'-N1	5.46	112.56	108.20
1	X	63	A	N1-C2-N3	-5.46	126.57	129.30
1	X	802	A	C4'-C3'-C2'	5.46	108.06	102.60
1	X	1943	A	C5'-C4'-C3'	-5.46	107.27	116.00
1	X	214	C	O4'-C1'-N1	5.45	112.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	773	G	OP1-P-O3'	5.45	117.20	105.20
1	X	1223	G	N3-C4-N9	5.45	129.27	126.00
1	X	615	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	2709	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	545	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	11	G	N7-C8-N9	5.45	115.82	113.10
1	X	774	A	N9-C4-C5	-5.45	103.62	105.80
1	X	1678	G	P-O3'-C3'	-5.45	113.16	119.70
1	X	1164	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	2440	C	O4'-C1'-N1	5.45	112.56	108.20
1	X	398	C	O4'-C1'-N1	5.44	112.56	108.20
1	X	1412	C	O4'-C1'-N1	5.44	112.55	108.20
1	X	56	C	O4'-C1'-N1	5.44	112.55	108.20
1	X	1635	G	C8-N9-C4	-5.44	104.22	106.40
1	X	1938	U	P-O5'-C5'	5.44	129.60	120.90
1	X	1963	G	O4'-C1'-N9	5.44	112.55	108.20
2	Y	5	C	N1-C2-O2	5.44	122.16	118.90
1	X	1500	U	O4'-C1'-N1	5.44	112.55	108.20
1	X	1935	A	P-O5'-C5'	-5.44	112.20	120.90
1	X	1421	U	O4'-C1'-N1	5.43	112.55	108.20
2	Y	32	C	O4'-C1'-N1	5.43	112.55	108.20
1	X	1286	U	O4'-C1'-N1	5.43	112.54	108.20
1	X	1975	G	N9-C1'-C2'	5.43	121.06	114.00
1	X	851	C	O4'-C1'-N1	5.43	112.54	108.20
1	X	1660	G	C4'-C3'-C2'	-5.43	97.17	102.60
1	X	2659	C	O4'-C1'-N1	5.42	112.54	108.20
1	X	242	A	C5'-C4'-C3'	5.42	124.68	116.00
1	X	1617	G	C5-C6-N1	5.42	114.21	111.50
1	X	2172	U	O4'-C1'-N1	5.42	112.54	108.20
1	X	1608	U	O4'-C1'-N1	5.42	112.54	108.20
1	X	2792	C	O4'-C1'-N1	5.42	112.54	108.20
2	Y	58	G	P-O3'-C3'	5.42	126.20	119.70
1	X	79	G	C8-N9-C4	-5.42	104.23	106.40
1	X	1821	A	O4'-C4'-C3'	-5.42	98.58	104.00
1	X	1695	U	O4'-C1'-N1	5.42	112.53	108.20
1	X	1927	U	P-O3'-C3'	5.42	126.20	119.70
1	X	2484	G	P-O5'-C5'	5.42	129.57	120.90
1	X	673	G	C4'-C3'-C2'	5.42	108.02	102.60
1	X	806	A	O4'-C1'-N9	-5.41	103.87	108.20
1	X	976	C	O4'-C1'-N1	5.41	112.53	108.20
1	X	1043	A	O4'-C1'-N9	5.41	112.53	108.20
1	X	1937	G	P-O3'-C3'	5.41	126.19	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	798	G	P-O3'-C3'	5.41	126.19	119.70
1	X	959	C	P-O3'-C3'	-5.41	113.21	119.70
1	X	2499	C	O4'-C1'-N1	5.41	112.53	108.20
1	X	11	G	C8-N9-C4	-5.41	104.24	106.40
1	X	923	A	N1-C6-N6	5.41	121.84	118.60
1	X	1077	U	P-O3'-C3'	5.41	126.19	119.70
1	X	2042	A	C4'-C3'-C2'	-5.41	97.19	102.60
2	Y	118	G	O4'-C1'-N9	5.41	112.53	108.20
1	X	1909	U	N1-C2-O2	5.40	126.58	122.80
1	X	2075	U	O4'-C1'-N1	5.40	112.52	108.20
1	X	2854	G	N7-C8-N9	5.40	115.80	113.10
1	X	479	G	N1-C6-O6	5.40	123.14	119.90
1	X	2323	U	P-O3'-C3'	5.40	126.18	119.70
1	X	2694	G	C5-C6-O6	-5.40	125.36	128.60
2	Y	17	A	P-O3'-C3'	5.39	126.17	119.70
1	X	157	G	C5'-C4'-C3'	-5.39	107.38	116.00
1	X	749	C	O4'-C1'-N1	5.39	112.51	108.20
2	Y	90	C	N1-C2-O2	5.39	122.13	118.90
1	X	430	C	C6-N1-C2	-5.38	118.15	120.30
1	X	1712	G	C4-N9-C1'	5.38	133.50	126.50
1	X	1986	G	N3-C4-C5	-5.38	125.91	128.60
1	X	2570	C	O4'-C1'-N1	5.38	112.51	108.20
1	X	175	C	C5-C6-N1	5.38	123.69	121.00
1	X	246	C	N1-C2-O2	5.38	122.13	118.90
1	X	1014	G	N3-C4-C5	-5.38	125.91	128.60
1	X	1490	U	O4'-C1'-N1	5.38	112.50	108.20
1	X	1385	C	N1-C2-O2	5.38	122.13	118.90
1	X	2015	G	N9-C1'-C2'	5.38	120.99	114.00
1	X	793	G	N1-C6-O6	-5.38	116.67	119.90
1	X	1036	G	P-O3'-C3'	5.38	126.15	119.70
1	X	2072	C	O4'-C1'-N1	5.38	112.50	108.20
1	X	2089	C	O4'-C1'-N1	5.38	112.50	108.20
1	X	941	U	O4'-C1'-N1	5.38	112.50	108.20
1	X	2492	G	N3-C4-C5	-5.38	125.91	128.60
1	X	184	A	O4'-C1'-N9	5.37	112.50	108.20
1	X	542	A	P-O3'-C3'	5.37	126.15	119.70
1	X	1139	A	O4'-C1'-C2'	-5.37	100.43	105.80
1	X	1467	U	O4'-C4'-C3'	-5.37	98.63	104.00
1	X	1685	A	P-O5'-C5'	5.37	129.50	120.90
2	Y	92	G	C3'-C2'-C1'	-5.37	97.20	101.50
1	X	467	U	C5'-C4'-C3'	5.37	124.59	116.00
1	X	1858	C	N1-C2-O2	5.37	122.12	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2403	C	N1-C2-O2	5.37	122.12	118.90
1	X	2717	G	O4'-C1'-N9	5.37	112.50	108.20
2	Y	29	C	O4'-C1'-N1	5.37	112.49	108.20
1	X	751	G	O5'-P-OP2	-5.37	100.87	105.70
1	X	1339	U	OP2-P-O3'	5.37	117.01	105.20
1	X	1715	A	P-O3'-C3'	5.37	126.14	119.70
1	X	2658	A	O5'-P-OP2	-5.37	100.87	105.70
1	X	213	C	O4'-C1'-N1	5.36	112.49	108.20
1	X	863	C	O4'-C1'-N1	5.36	112.49	108.20
1	X	99	U	N3-C2-O2	-5.36	118.45	122.20
1	X	682	G	C3'-C2'-C1'	5.36	105.79	101.50
1	X	2232	G	C5-C6-O6	-5.36	125.38	128.60
1	X	2691	C	N3-C2-O2	-5.36	118.15	121.90
1	X	308	C	P-O3'-C3'	-5.36	113.27	119.70
1	X	1497	C	C6-N1-C2	-5.36	118.16	120.30
1	X	1840	A	O4'-C1'-N9	5.36	112.48	108.20
1	X	235	C	N1-C2-O2	5.36	122.11	118.90
1	X	513	A	C1'-O4'-C4'	-5.36	105.61	109.90
1	X	2666	U	C3'-C2'-C1'	5.36	105.78	101.50
1	X	472	C	O4'-C1'-N1	5.35	112.48	108.20
1	X	1219	C	O4'-C1'-N1	5.35	112.48	108.20
1	X	1222	G	P-O3'-C3'	5.35	126.12	119.70
1	X	1491	C	O4'-C1'-N1	5.35	112.48	108.20
1	X	319	G	C5-C6-O6	-5.35	125.39	128.60
1	X	814	G	N9-C1'-C2'	5.35	120.95	114.00
1	X	1199	U	O4'-C1'-N1	5.35	112.48	108.20
1	X	1390	G	N3-C4-C5	-5.35	125.93	128.60
1	X	2483	U	O4'-C1'-N1	5.35	112.48	108.20
1	X	2870	C	C6-N1-C2	-5.35	118.16	120.30
1	X	1803	G	O4'-C1'-N9	5.34	112.48	108.20
1	X	1622	G	N3-C4-C5	-5.34	125.93	128.60
1	X	417	C	N1-C2-O2	5.34	122.10	118.90
1	X	2410	U	OP2-P-O3'	5.34	116.95	105.20
1	X	2688	G	P-O3'-C3'	-5.34	113.29	119.70
1	X	1172	U	O4'-C1'-N1	5.34	112.47	108.20
1	X	1496	G	O4'-C1'-N9	5.34	112.47	108.20
1	X	1753	A	C8-N9-C4	-5.34	103.67	105.80
1	X	2553	G	N7-C8-N9	5.34	115.77	113.10
1	X	2700	U	OP1-P-O3'	5.34	116.94	105.20
1	X	458	G	C3'-C2'-C1'	5.33	105.77	101.50
1	X	694	G	O4'-C1'-N9	5.33	112.47	108.20
1	X	1283	C	N3-C4-C5	-5.33	119.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1711	C	P-O3'-C3'	5.33	126.10	119.70
1	X	1278	A	C5-N7-C8	-5.33	101.23	103.90
1	X	1882	G	O4'-C1'-N9	5.33	112.47	108.20
1	X	2535	C	N1-C2-O2	5.33	122.10	118.90
2	Y	101	A	C3'-C2'-C1'	-5.33	97.24	101.50
1	X	70	A	P-O5'-C5'	-5.33	112.38	120.90
1	X	1790	G	C2'-C3'-O3'	5.33	122.22	113.70
1	X	2774	U	P-O3'-C3'	5.33	126.09	119.70
2	Y	10	U	O4'-C4'-C3'	-5.33	98.67	104.00
11	I	44	GLY	N-CA-C	5.33	126.42	113.10
1	X	757	U	P-O3'-C3'	5.33	126.09	119.70
1	X	1720	G	P-O3'-C3'	-5.33	113.31	119.70
1	X	1301	U	N3-C2-O2	-5.33	118.47	122.20
1	X	2429	A	P-O3'-C3'	-5.33	113.31	119.70
2	Y	12	C	O4'-C4'-C3'	-5.33	98.67	104.00
1	X	973	U	O3'-P-O5'	-5.32	93.89	104.00
1	X	1722	G	O4'-C1'-N9	5.32	112.46	108.20
1	X	61	U	C1'-O4'-C4'	-5.32	105.65	109.90
1	X	1225	G	N9-C1'-C2'	5.32	120.91	114.00
1	X	1785	A	O4'-C1'-N9	5.32	112.45	108.20
2	Y	55	C	P-O3'-C3'	5.32	126.08	119.70
1	X	858	G	P-O3'-C3'	5.32	126.08	119.70
1	X	1202	U	O4'-C1'-N1	5.32	112.45	108.20
1	X	2375	G	O4'-C4'-C3'	-5.32	98.69	104.00
1	X	2732	C	N1-C2-O2	5.32	122.09	118.90
23	U	32	ARG	N-CA-C	-5.31	96.65	111.00
1	X	1716	G	C1'-O4'-C4'	5.31	114.15	109.90
1	X	2015	G	C5-C6-N1	5.31	114.16	111.50
1	X	1238	A	O4'-C1'-N9	5.31	112.45	108.20
1	X	1725	C	P-O3'-C3'	5.31	126.07	119.70
1	X	524	A	O4'-C4'-C3'	-5.31	98.69	104.00
1	X	146	C	O4'-C1'-N1	5.30	112.44	108.20
1	X	2275	U	P-O5'-C5'	5.30	129.39	120.90
1	X	536	A	C3'-C2'-C1'	5.30	105.74	101.50
1	X	1056	U	P-O3'-C3'	5.30	126.06	119.70
1	X	1248	G	O3'-P-O5'	-5.30	93.93	104.00
1	X	876	A	P-O3'-C3'	5.30	126.06	119.70
1	X	1210	C	O4'-C1'-N1	5.30	112.44	108.20
1	X	2691	C	N1-C2-O2	5.30	122.08	118.90
1	X	418	C	P-O5'-C5'	5.30	129.37	120.90
1	X	1661	C	C4'-C3'-C2'	-5.30	97.30	102.60
1	X	2071	G	O4'-C1'-N9	5.30	112.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2568	A	O4'-C1'-N9	5.30	112.44	108.20
1	X	33	C	N1-C2-O2	5.29	122.08	118.90
1	X	1988	A	C5-N7-C8	-5.29	101.25	103.90
1	X	179	U	O4'-C1'-N1	5.29	112.44	108.20
1	X	723	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	2256	G	N7-C8-N9	5.29	115.75	113.10
2	Y	90	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	817	A	O4'-C1'-N9	5.29	112.43	108.20
1	X	2321	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	2551	A	OP1-P-O3'	5.29	116.84	105.20
1	X	851	C	C3'-C2'-C1'	-5.29	97.27	101.50
1	X	2567	G	N3-C4-C5	-5.29	125.96	128.60
1	X	2804	G	C5-C6-O6	-5.29	125.43	128.60
1	X	2229	G	C2-N3-C4	5.29	114.54	111.90
1	X	98	U	O4'-C1'-N1	5.29	112.43	108.20
1	X	427	C	O4'-C1'-N1	5.29	112.43	108.20
1	X	1154	A	C4'-C3'-C2'	5.29	107.89	102.60
1	X	2667	C	N1-C2-O2	5.29	122.07	118.90
1	X	329	C	O4'-C1'-N1	5.28	112.43	108.20
1	X	554	U	C3'-C2'-C1'	-5.28	97.27	101.50
1	X	1054	C	O4'-C1'-N1	5.28	112.43	108.20
1	X	1496	G	C4'-C3'-O3'	5.28	123.57	113.00
1	X	2418	A	C3'-C2'-C1'	5.28	105.73	101.50
1	X	2854	G	C5-N7-C8	-5.28	101.66	104.30
1	X	969	U	C4'-C3'-C2'	5.28	107.88	102.60
1	X	1746	A	N1-C6-N6	-5.28	115.43	118.60
1	X	2464	G	C3'-C2'-C1'	-5.28	97.28	101.50
1	X	337	G	N7-C8-N9	5.28	115.74	113.10
1	X	4	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	664	C	O4'-C1'-N1	5.28	112.42	108.20
1	X	1741	G	C8-N9-C4	-5.28	104.29	106.40
1	X	1987	G	N3-C4-C5	-5.28	125.96	128.60
1	X	2276	C	O4'-C1'-N1	5.28	112.42	108.20
2	Y	86	A	N1-C6-N6	5.28	121.77	118.60
1	X	1863	U	O4'-C1'-N1	5.27	112.42	108.20
1	X	346	C	C2-N3-C4	5.27	122.54	119.90
1	X	1841	G	C8-N9-C4	-5.27	104.29	106.40
1	X	78	C	C6-N1-C2	-5.27	118.19	120.30
1	X	352	G	P-O5'-C5'	5.27	129.33	120.90
1	X	1326	U	C2-N1-C1'	5.27	124.02	117.70
1	X	1341	G	C5-C6-N1	5.27	114.14	111.50
1	X	746	G	N3-C4-N9	5.27	129.16	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1263	G	P-O3'-C3'	5.27	126.02	119.70
1	X	1873	A	O4'-C1'-N9	5.27	112.41	108.20
1	X	2568	A	O4'-C4'-C3'	-5.27	98.73	104.00
2	Y	107	C	N1-C2-O2	5.27	122.06	118.90
1	X	927	C	N1-C2-O2	5.26	122.06	118.90
1	X	1980	A	C4-C5-C6	5.26	119.63	117.00
2	Y	97	C	O4'-C1'-N1	5.26	112.41	108.20
1	X	358	C	C5-C6-N1	5.26	123.63	121.00
1	X	1478	U	N3-C2-O2	-5.26	118.52	122.20
1	X	1755	G	O5'-P-OP2	-5.26	100.97	105.70
1	X	2047	C	O4'-C1'-N1	5.26	112.41	108.20
1	X	1194	U	C2'-C3'-O3'	5.26	122.11	113.70
1	X	2479	U	O4'-C1'-N1	5.26	112.41	108.20
1	X	2564	U	O4'-C1'-N1	5.26	112.41	108.20
1	X	617	U	C2-N1-C1'	5.26	124.01	117.70
1	X	1657	A	C5'-C4'-O4'	-5.26	102.79	109.10
1	X	2000	U	O4'-C1'-N1	5.26	112.41	108.20
1	X	765	C	N1-C2-O2	5.25	122.05	118.90
1	X	1703	C	O4'-C1'-N1	5.25	112.40	108.20
1	X	1923	U	P-O3'-C3'	5.25	126.00	119.70
1	X	2380	U	O4'-C1'-N1	5.25	112.40	108.20
1	X	940	G	O4'-C1'-N9	5.25	112.40	108.20
1	X	954	U	C5-C4-O4	-5.25	122.75	125.90
1	X	1687	C	P-O3'-C3'	5.25	126.00	119.70
1	X	2524	G	C8-N9-C4	-5.25	104.30	106.40
1	X	320	A	O4'-C1'-N9	5.25	112.40	108.20
1	X	1458	A	P-O3'-C3'	5.25	126.00	119.70
2	Y	41	A	P-O3'-C3'	5.25	126.00	119.70
13	K	11	ASN	C-N-CA	5.25	134.81	121.70
1	X	949	G	C3'-C2'-C1'	-5.24	97.31	101.50
1	X	1432	G	C1'-O4'-C4'	-5.24	105.70	109.90
1	X	2826	C	P-O3'-C3'	5.24	125.99	119.70
1	X	133	C	N1-C2-O2	5.24	122.05	118.90
1	X	2481	G	P-O3'-C3'	5.24	125.99	119.70
1	X	1201	G	P-O3'-C3'	5.24	125.99	119.70
1	X	2422	C	N3-C4-C5	5.24	124.00	121.90
1	X	1830	C	N1-C1'-C2'	5.24	120.81	114.00
1	X	2773	G	P-O3'-C3'	5.24	125.98	119.70
1	X	884	C	O4'-C1'-N1	5.24	112.39	108.20
1	X	1765	C	N3-C2-O2	-5.24	118.23	121.90
15	M	29	PRO	N-CA-C	5.24	125.72	112.10
1	X	1231	A	O4'-C1'-N9	5.24	112.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1273	G	C5-C6-O6	-5.24	125.46	128.60
1	X	1278	A	N7-C8-N9	5.24	116.42	113.80
1	X	1663	C	O3'-P-O5'	-5.24	94.05	104.00
1	X	2014	A	C4'-C3'-C2'	5.24	107.84	102.60
1	X	2848	A	C1'-O4'-C4'	-5.24	105.71	109.90
1	X	1811	A	C4'-C3'-C2'	5.23	107.83	102.60
1	X	2039	G	N3-C2-N2	-5.23	116.24	119.90
1	X	169	C	O5'-P-OP2	-5.23	100.99	105.70
1	X	1338	G	C2-N3-C4	5.23	114.51	111.90
1	X	1326	U	N1-C2-O2	5.22	126.46	122.80
1	X	2662	C	N1-C2-O2	5.22	122.03	118.90
2	Y	63	A	O4'-C1'-N9	5.22	112.38	108.20
4	B	162	MET	CB-CA-C	5.22	120.84	110.40
1	X	985	G	N7-C8-N9	5.22	115.71	113.10
1	X	542	A	N1-C6-N6	5.22	121.73	118.60
1	X	967	G	P-O5'-C5'	5.22	129.25	120.90
1	X	1446	U	O4'-C1'-N1	5.22	112.38	108.20
1	X	1764	A	C5-C6-N6	-5.22	119.53	123.70
1	X	2209	G	C8-N9-C4	-5.22	104.31	106.40
1	X	1235	C	C6-N1-C2	-5.22	118.21	120.30
1	X	2619	G	C8-N9-C4	-5.22	104.31	106.40
1	X	245	C	N1-C2-O2	5.21	122.03	118.90
1	X	480	G	C6-C5-N7	-5.21	127.27	130.40
1	X	559	C	C5'-C4'-O4'	5.21	115.36	109.10
1	X	825	C	C5'-C4'-O4'	5.21	115.36	109.10
1	X	2190	A	C4'-C3'-C2'	-5.21	97.39	102.60
1	X	2488	G	C5-C6-N1	5.21	114.11	111.50
1	X	468	A	P-O3'-C3'	5.21	125.95	119.70
1	X	617	U	N1-C2-O2	5.21	126.45	122.80
1	X	2243	C	O4'-C1'-N1	5.21	112.37	108.20
1	X	483	A	O5'-C5'-C4'	5.21	121.60	111.70
1	X	1637	U	O4'-C1'-N1	5.21	112.37	108.20
1	X	2473	G	N3-C4-C5	-5.21	125.99	128.60
1	X	2605	C	O4'-C1'-N1	5.21	112.37	108.20
1	X	1885	C	O4'-C1'-N1	5.21	112.37	108.20
1	X	542	A	C5-C6-N6	-5.21	119.53	123.70
1	X	799	C	P-O3'-C3'	5.21	125.95	119.70
1	X	1877	C	O4'-C1'-N1	5.21	112.36	108.20
1	X	2284	U	O4'-C1'-N1	5.21	112.36	108.20
1	X	2448	A	O4'-C1'-N9	5.21	112.37	108.20
2	Y	41	A	O4'-C1'-N9	5.21	112.36	108.20
1	X	1729	C	O4'-C1'-N1	5.21	112.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2349	G	C3'-C2'-C1'	-5.21	97.34	101.50
1	X	945	G	C8-N9-C4	-5.20	104.32	106.40
1	X	1631	C	C4'-C3'-C2'	-5.20	97.40	102.60
1	X	593	C	P-O5'-C5'	5.20	129.22	120.90
1	X	1629	G	P-O3'-C3'	5.20	125.94	119.70
2	Y	53	G	C8-N9-C4	-5.20	104.32	106.40
1	X	542	A	C5'-C4'-O4'	5.20	115.34	109.10
1	X	560	G	P-O3'-C3'	-5.20	113.46	119.70
1	X	2441	U	O4'-C1'-N1	5.20	112.36	108.20
1	X	2697	G	C5-C6-O6	-5.20	125.48	128.60
1	X	2018	G	O4'-C1'-C2'	-5.20	100.60	105.80
1	X	2408	G	C2'-C3'-O3'	5.20	122.02	113.70
1	X	2013	A	C1'-O4'-C4'	-5.20	105.74	109.90
1	X	349	G	P-O5'-C5'	5.20	129.21	120.90
1	X	1142	G	C5-C6-O6	-5.20	125.48	128.60
1	X	1336	G	N9-C4-C5	-5.20	103.32	105.40
1	X	1699	A	O4'-C1'-N9	-5.20	104.04	108.20
1	X	1747	G	N9-C1'-C2'	5.20	120.75	114.00
1	X	1963	G	C8-N9-C4	-5.20	104.32	106.40
1	X	2471	U	O4'-C1'-N1	5.20	112.36	108.20
1	X	2573	C	O4'-C1'-N1	5.20	112.36	108.20
1	X	2854	G	P-O5'-C5'	5.20	129.21	120.90
1	X	596	C	P-O3'-C3'	5.19	125.93	119.70
1	X	2810	A	C1'-O4'-C4'	-5.19	105.74	109.90
1	X	1613	G	O4'-C1'-N9	5.19	112.35	108.20
2	Y	54	U	C5'-C4'-O4'	5.19	115.33	109.10
1	X	874	A	O4'-C1'-N9	5.19	112.35	108.20
1	X	2560	G	C8-N9-C4	-5.19	104.32	106.40
1	X	499	G	O4'-C1'-N9	5.19	112.35	108.20
1	X	956	A	C5'-C4'-O4'	5.19	115.33	109.10
1	X	1626	A	N1-C2-N3	-5.19	126.71	129.30
1	X	2377	U	O4'-C1'-N1	5.19	112.35	108.20
1	X	18	U	P-O3'-C3'	-5.19	113.48	119.70
1	X	786	U	O4'-C1'-N1	5.19	112.35	108.20
1	X	97	U	C5'-C4'-C3'	-5.18	107.70	116.00
1	X	2489	C	P-O3'-C3'	-5.18	113.48	119.70
1	X	2799	C	N3-C4-C5	5.18	123.97	121.90
1	X	78	C	C5-C6-N1	5.18	123.59	121.00
1	X	422	C	C6-N1-C2	-5.18	118.23	120.30
1	X	1496	G	C8-N9-C4	-5.18	104.33	106.40
11	I	35	LYS	N-CA-C	-5.18	97.02	111.00
1	X	2858	A	P-O5'-C5'	5.18	129.19	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	646	C	C6-N1-C2	-5.18	118.23	120.30
1	X	751	G	C3'-C2'-C1'	-5.18	97.36	101.50
11	I	64	GLY	N-CA-C	5.18	126.04	113.10
1	X	230	C	O4'-C1'-N1	5.17	112.34	108.20
1	X	1396	C	O4'-C1'-N1	5.17	112.34	108.20
1	X	246	C	N3-C2-O2	-5.17	118.28	121.90
1	X	309	G	C5-C6-O6	-5.17	125.50	128.60
1	X	330	C	N1-C2-O2	5.17	122.00	118.90
1	X	2543	A	O4'-C1'-N9	5.17	112.34	108.20
1	X	341	A	C3'-C2'-C1'	5.17	105.64	101.50
1	X	1170	U	O4'-C1'-N1	5.17	112.33	108.20
1	X	2790	C	O4'-C1'-N1	5.17	112.33	108.20
1	X	1038	U	O4'-C1'-N1	5.17	112.33	108.20
1	X	1112	U	O4'-C1'-N1	5.17	112.33	108.20
1	X	1150	C	O4'-C1'-N1	5.17	112.33	108.20
1	X	1825	C	C3'-C2'-C1'	-5.17	97.37	101.50
1	X	351	A	C3'-C2'-C1'	-5.16	97.37	101.50
1	X	1717	A	C5-C6-N1	5.16	120.28	117.70
1	X	2237	C	O4'-C1'-N1	5.16	112.33	108.20
1	X	2385	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2493	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2705	A	C4'-C3'-O3'	5.16	123.33	113.00
1	X	2855	C	O4'-C1'-N1	5.16	112.33	108.20
1	X	454	G	P-O3'-C3'	5.16	125.89	119.70
1	X	1711	C	P-O5'-C5'	5.16	129.16	120.90
1	X	2776	U	P-O3'-C3'	5.16	125.89	119.70
1	X	200	A	P-O3'-C3'	5.16	125.89	119.70
1	X	1014	G	C2-N3-C4	5.16	114.48	111.90
1	X	1281	A	OP2-P-O3'	5.16	116.55	105.20
1	X	823	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2650	G	C4'-C3'-C2'	5.16	107.76	102.60
1	X	2766	U	O4'-C1'-N1	5.16	112.33	108.20
1	X	2786	G	O4'-C1'-N9	5.16	112.32	108.20
1	X	951	G	O4'-C4'-C3'	-5.15	98.85	104.00
1	X	1124	U	O4'-C1'-N1	5.15	112.32	108.20
1	X	1623	C	P-O3'-C3'	5.15	125.88	119.70
1	X	2593	A	O3'-P-O5'	-5.15	94.21	104.00
1	X	730	C	O4'-C1'-N1	5.15	112.32	108.20
1	X	1469	U	N1-C2-N3	5.15	117.99	114.90
1	X	1265	G	O5'-P-OP1	5.15	116.88	110.70
3	A	248	THR	CB-CA-C	5.15	125.50	111.60
1	X	72	A	O4'-C1'-N9	5.15	112.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1390	G	C8-N9-C4	-5.15	104.34	106.40
1	X	1987	G	C8-N9-C4	-5.15	104.34	106.40
1	X	1250	A	P-O3'-C3'	5.14	125.87	119.70
1	X	1622	G	P-O3'-C3'	5.14	125.87	119.70
1	X	1940	C	O4'-C1'-N1	5.14	112.32	108.20
1	X	1429	A	N9-C1'-C2'	5.14	120.68	114.00
1	X	1912	G	P-O3'-C3'	5.14	125.87	119.70
1	X	2039	G	N7-C8-N9	5.14	115.67	113.10
2	Y	53	G	N3-C4-C5	-5.14	126.03	128.60
1	X	70	A	C5'-C4'-C3'	-5.14	107.77	116.00
1	X	2561	G	C5-C6-O6	-5.14	125.52	128.60
1	X	1648	C	N1-C2-O2	5.14	121.98	118.90
1	X	2274	C	C6-N1-C2	-5.14	118.24	120.30
1	X	1790	G	C4'-C3'-C2'	5.14	107.74	102.60
1	X	2663	U	P-O3'-C3'	-5.14	113.53	119.70
1	X	1014	G	C8-N9-C4	-5.14	104.35	106.40
1	X	1167	A	O4'-C1'-N9	-5.14	104.09	108.20
9	G	106	TYR	CA-C-N	-5.14	105.90	117.20
1	X	582	G	P-O3'-C3'	5.13	125.86	119.70
1	X	771	C	N1-C2-O2	5.13	121.98	118.90
1	X	955	G	C4-N9-C1'	5.13	133.18	126.50
1	X	1248	G	OP1-P-O3'	5.13	116.49	105.20
11	I	32	ARG	N-CA-C	-5.13	97.14	111.00
1	X	626	A	P-O3'-C3'	5.13	125.86	119.70
1	X	2298	U	C4'-C3'-C2'	5.13	107.73	102.60
1	X	1975	G	C2-N3-C4	5.13	114.47	111.90
1	X	2697	G	N3-C4-C5	-5.13	126.04	128.60
1	X	2855	C	C6-N1-C2	-5.13	118.25	120.30
1	X	2176	U	O4'-C1'-N1	5.13	112.30	108.20
1	X	2279	G	C8-N9-C4	-5.13	104.35	106.40
2	Y	10	U	O4'-C1'-N1	5.12	112.30	108.20
1	X	1432	G	P-O3'-C3'	5.12	125.85	119.70
1	X	240	U	O4'-C4'-C3'	-5.12	98.88	104.00
1	X	984	A	P-O3'-C3'	5.12	125.84	119.70
1	X	2681	A	C4'-C3'-C2'	-5.12	97.48	102.60
1	X	820	U	O4'-C1'-N1	5.12	112.30	108.20
1	X	1409	U	C1'-O4'-C4'	-5.12	105.81	109.90
1	X	2011	U	C5-C4-O4	-5.12	122.83	125.90
1	X	2619	G	C5'-C4'-C3'	-5.12	107.81	116.00
1	X	2846	G	O5'-P-OP2	-5.12	101.09	105.70
1	X	2296	U	O4'-C1'-N1	5.12	112.29	108.20
1	X	2804	G	C6-N1-C2	-5.12	122.03	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1279	G	C1'-O4'-C4'	-5.12	105.81	109.90
1	X	577	U	C2-N3-C4	5.11	130.07	127.00
1	X	2867	G	C3'-C2'-C1'	5.11	105.59	101.50
2	Y	8	C	O4'-C1'-N1	5.11	112.29	108.20
1	X	1351	G	C3'-C2'-C1'	5.11	105.59	101.50
1	X	660	G	C8-N9-C4	-5.11	104.36	106.40
1	X	2006	G	C5'-C4'-O4'	5.11	115.23	109.10
10	H	26	ASN	C-N-CA	5.11	134.47	121.70
12	J	88	LYS	N-CA-C	5.11	124.80	111.00
1	X	1559	G	P-O3'-C3'	5.11	125.83	119.70
1	X	1712	G	C8-N9-C1'	-5.11	120.36	127.00
1	X	225	G	O4'-C1'-N9	5.11	112.28	108.20
1	X	1407	G	C4-N9-C1'	5.11	133.14	126.50
1	X	1627	C	O4'-C1'-N1	5.11	112.28	108.20
1	X	1853	C	O4'-C1'-N1	5.11	112.28	108.20
4	B	132	LYS	C-N-CA	5.11	134.46	121.70
1	X	1244	U	C5-C6-N1	5.10	125.25	122.70
1	X	1218	C	O4'-C1'-N1	5.10	112.28	108.20
1	X	1468	A	N1-C6-N6	-5.10	115.54	118.60
1	X	327	C	N1-C2-O2	5.10	121.96	118.90
1	X	334	G	C2-N3-C4	5.10	114.45	111.90
1	X	519	C	C5-C6-N1	5.10	123.55	121.00
1	X	1142	G	P-O3'-C3'	5.10	125.82	119.70
1	X	1245	G	O4'-C1'-N9	5.10	112.28	108.20
1	X	1733	U	O4'-C1'-N1	5.10	112.28	108.20
1	X	1679	U	N1-C2-N3	5.10	117.96	114.90
1	X	2196	U	O4'-C1'-N1	5.10	112.28	108.20
1	X	579	G	C5-N7-C8	5.10	106.85	104.30
1	X	1340	C	O3'-P-O5'	-5.10	94.32	104.00
1	X	561	U	C3'-C2'-C1'	-5.09	97.42	101.50
1	X	1120	C	C3'-C2'-C1'	5.09	105.58	101.50
1	X	2659	C	P-O5'-C5'	5.09	129.05	120.90
1	X	132	U	O4'-C1'-N1	5.09	112.28	108.20
1	X	34	U	C5'-C4'-O4'	5.09	115.21	109.10
1	X	485	G	P-O5'-C5'	5.09	129.04	120.90
1	X	523	A	N9-C1'-C2'	5.09	120.62	114.00
1	X	1237	G	O4'-C1'-N9	5.09	112.27	108.20
1	X	2396	C	P-O5'-C5'	-5.09	112.76	120.90
1	X	2476	A	P-O3'-C3'	5.09	125.81	119.70
1	X	2650	G	N3-C4-C5	-5.09	126.06	128.60
1	X	345	U	P-O5'-C5'	5.09	129.04	120.90
1	X	206	U	N1-C2-O2	5.09	126.36	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	759	C	O5'-C5'-C4'	5.09	121.37	111.70
1	X	993	C	P-O3'-C3'	-5.09	113.60	119.70
1	X	1497	C	C5-C6-N1	5.09	123.54	121.00
1	X	2680	U	O4'-C1'-N1	5.09	112.27	108.20
1	X	2784	A	O4'-C1'-N9	-5.08	104.13	108.20
1	X	2794	G	P-O5'-C5'	-5.08	112.76	120.90
3	A	242	ALA	N-CA-C	5.08	124.73	111.00
1	X	2416	U	C3'-C2'-C1'	-5.08	97.43	101.50
1	X	2827	G	N3-C4-C5	-5.08	126.06	128.60
1	X	2867	G	C5'-C4'-O4'	5.08	115.20	109.10
2	Y	28	A	C2-N3-C4	5.08	113.14	110.60
1	X	1944	C	N1-C2-O2	5.08	121.95	118.90
1	X	1994	U	O4'-C1'-N1	5.08	112.27	108.20
1	X	2487	G	C8-N9-C4	-5.08	104.37	106.40
1	X	2620	G	C5-C6-O6	-5.08	125.55	128.60
1	X	551	A	C3'-C2'-C1'	-5.08	97.44	101.50
1	X	639	G	C5-C6-O6	-5.08	125.55	128.60
1	X	811	G	O4'-C1'-N9	5.08	112.26	108.20
1	X	2299	A	N9-C1'-C2'	5.08	120.60	114.00
1	X	2314	A	P-O5'-C5'	5.08	129.03	120.90
1	X	2632	U	P-O3'-C3'	5.08	125.79	119.70
1	X	1994	U	OP1-P-O3'	5.08	116.36	105.20
1	X	71	A	P-O5'-C5'	5.07	129.02	120.90
1	X	812	G	C8-N9-C4	-5.07	104.37	106.40
1	X	1695	U	N3-C2-O2	-5.07	118.65	122.20
1	X	2229	G	N9-C4-C5	5.07	107.43	105.40
1	X	70	A	P-O3'-C3'	5.07	125.78	119.70
1	X	777	A	C5'-C4'-C3'	-5.07	107.89	116.00
1	X	773	G	O4'-C1'-N9	5.07	112.25	108.20
1	X	1753	A	N7-C8-N9	5.07	116.33	113.80
1	X	1264	C	N1-C2-O2	5.07	121.94	118.90
1	X	1509	A	P-O5'-C5'	5.07	129.01	120.90
1	X	69	G	O4'-C1'-N9	5.07	112.25	108.20
1	X	1973	C	O4'-C1'-N1	5.07	112.25	108.20
1	X	2681	A	C6-N1-C2	-5.07	115.56	118.60
1	X	1099	A	C3'-C2'-C1'	5.06	105.55	101.50
1	X	1528	C	C5-C6-N1	5.06	123.53	121.00
1	X	1223	G	C5-C6-O6	-5.06	125.56	128.60
1	X	2251	U	P-O3'-C3'	5.06	125.77	119.70
1	X	2487	G	C5-C6-N1	5.06	114.03	111.50
1	X	1524	C	O4'-C1'-N1	5.06	112.25	108.20
1	X	1928	G	P-O5'-C5'	5.06	128.99	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2324	G	N3-C4-C5	-5.06	126.07	128.60
5	C	163	ASN	C-N-CA	5.06	134.34	121.70
1	X	664	C	N1-C2-O2	5.06	121.93	118.90
1	X	2485	U	P-O3'-C3'	5.06	125.77	119.70
1	X	2731	G	O4'-C1'-N9	5.06	112.25	108.20
1	X	26	G	C5-C6-O6	-5.05	125.57	128.60
1	X	559	C	N3-C2-O2	-5.05	118.36	121.90
1	X	1451	C	C5'-C4'-O4'	5.05	115.16	109.10
1	X	1674	C	C5'-C4'-O4'	-5.05	103.04	109.10
1	X	1796	A	C2-N3-C4	5.05	113.13	110.60
1	X	1799	A	C5'-C4'-O4'	5.05	115.16	109.10
1	X	2744	A	P-O3'-C3'	5.05	125.76	119.70
1	X	624	A	O4'-C1'-N9	5.05	112.24	108.20
1	X	1250	A	O4'-C1'-N9	-5.05	104.16	108.20
1	X	1666	G	O4'-C4'-C3'	-5.05	98.95	104.00
1	X	2064	U	O4'-C1'-N1	5.05	112.24	108.20
1	X	2288	A	P-O3'-C3'	5.05	125.76	119.70
1	X	2426	G	C1'-O4'-C4'	-5.05	105.86	109.90
1	X	461	A	C2-N3-C4	5.05	113.12	110.60
1	X	536	A	N1-C6-N6	5.05	121.63	118.60
1	X	635	C	C6-N1-C2	-5.05	118.28	120.30
1	X	1986	G	N1-C6-O6	-5.05	116.87	119.90
1	X	1665	C	O5'-P-OP2	-5.05	101.16	105.70
1	X	2507	U	P-O3'-C3'	5.05	125.75	119.70
1	X	1426	U	O4'-C1'-N1	5.04	112.24	108.20
1	X	1497	C	O4'-C1'-N1	5.04	112.23	108.20
1	X	1535	C	O4'-C1'-N1	5.04	112.23	108.20
1	X	1282	A	C5'-C4'-C3'	-5.04	107.93	116.00
1	X	1980	A	O4'-C1'-N9	5.04	112.23	108.20
1	X	2729	A	O4'-C1'-N9	5.04	112.23	108.20
1	X	1284	G	N7-C8-N9	5.04	115.62	113.10
1	X	769	C	O4'-C1'-N1	5.04	112.23	108.20
1	X	1199	U	OP2-P-O3'	5.04	116.28	105.20
1	X	1467	U	C1'-O4'-C4'	5.04	113.93	109.90
1	X	1838	G	P-O3'-C3'	5.04	125.75	119.70
1	X	337	G	C5-C6-O6	-5.04	125.58	128.60
1	X	407	A	O4'-C1'-N9	5.04	112.23	108.20
1	X	753	U	P-O3'-C3'	5.04	125.74	119.70
1	X	2745	A	N1-C2-N3	-5.04	126.78	129.30
1	X	107	G	C5'-C4'-C3'	-5.04	107.94	116.00
1	X	1872	A	C4'-C3'-C2'	-5.04	97.56	102.60
1	X	349	G	N3-C4-C5	-5.03	126.08	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	964	A	C5'-C4'-O4'	5.03	115.14	109.10
1	X	1291	G	O4'-C4'-C3'	-5.03	98.97	104.00
1	X	465	C	P-O5'-C5'	-5.03	112.85	120.90
1	X	1229	C	O4'-C1'-N1	5.03	112.22	108.20
1	X	2691	C	O3'-P-O5'	-5.03	94.44	104.00
1	X	17	G	P-O3'-C3'	-5.03	113.67	119.70
1	X	467	U	C5'-C4'-O4'	5.03	115.14	109.10
1	X	2228	U	N3-C4-O4	5.03	122.92	119.40
1	X	228	A	OP1-P-O3'	5.03	116.26	105.20
1	X	616	U	C5'-C4'-C3'	-5.03	107.96	116.00
1	X	1000	G	O4'-C1'-N9	5.03	112.22	108.20
1	X	1033	G	C5'-C4'-O4'	-5.03	103.07	109.10
1	X	1669	A	C3'-C2'-C1'	-5.03	97.48	101.50
1	X	1766	U	C5-C4-O4	-5.03	122.88	125.90
1	X	190	A	C1'-O4'-C4'	-5.03	105.88	109.90
1	X	560	G	C4'-C3'-C2'	5.03	107.63	102.60
1	X	633	G	P-O5'-C5'	5.03	128.94	120.90
1	X	1174	G	O4'-C1'-N9	5.03	112.22	108.20
1	X	1812	U	P-O5'-C5'	5.03	128.94	120.90
1	X	2503	G	C5-C6-N1	5.03	114.01	111.50
1	X	2567	G	C6-N1-C2	-5.03	122.08	125.10
1	X	2598	C	N3-C4-C5	5.03	123.91	121.90
1	X	2620	G	C4'-C3'-C2'	-5.03	97.57	102.60
1	X	767	G	P-O5'-C5'	5.02	128.94	120.90
1	X	1541	G	O4'-C1'-N9	5.02	112.22	108.20
1	X	2701	A	P-O3'-C3'	-5.02	113.67	119.70
1	X	2727	G	O4'-C1'-N9	5.02	112.22	108.20
1	X	1222	G	N3-C4-N9	5.02	129.01	126.00
1	X	1777	A	C1'-O4'-C4'	-5.02	105.88	109.90
1	X	2737	A	C5'-C4'-C3'	-5.02	107.97	116.00
2	Y	35	C	O4'-C1'-N1	5.02	112.22	108.20
1	X	232	A	P-O5'-C5'	5.02	128.93	120.90
1	X	344	G	C8-N9-C4	-5.02	104.39	106.40
1	X	480	G	N1-C6-O6	5.02	122.91	119.90
1	X	537	C	C3'-C2'-C1'	-5.01	97.49	101.50
1	X	573	C	N1-C2-O2	5.01	121.91	118.90
1	X	1049	C	O4'-C1'-N1	5.01	112.21	108.20
1	X	1669	A	C1'-O4'-C4'	-5.01	105.89	109.90
2	Y	54	U	C1'-O4'-C4'	-5.01	105.89	109.90
1	X	845	U	N3-C2-O2	-5.01	118.69	122.20
1	X	2261	G	C4'-C3'-C2'	5.01	107.61	102.60
1	X	73	A	N9-C1'-C2'	5.01	120.51	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	610	G	O3'-P-O5'	-5.01	94.48	104.00
1	X	1234	C	O4'-C1'-N1	5.01	112.21	108.20
1	X	1770	U	C4-C5-C6	5.01	122.71	119.70
1	X	1418	C	N1-C2-O2	5.01	121.91	118.90
1	X	497	C	C3'-C2'-C1'	-5.01	97.50	101.50
1	X	2340	C	OP1-P-OP2	5.01	127.11	119.60
1	X	1280	U	N1-C1'-C2'	5.00	120.51	114.00
1	X	1812	U	C2-N1-C1'	5.00	123.71	117.70
1	X	2347	C	C3'-C2'-C1'	-5.00	97.50	101.50
2	Y	45	C	N3-C2-O2	-5.00	118.40	121.90
1	X	1075	C	C3'-C2'-C1'	5.00	105.50	101.50
1	X	1671	A	OP1-P-OP2	5.00	127.10	119.60
1	X	1822	C	C3'-C2'-C1'	-5.00	97.50	101.50
1	X	2292	C	O4'-C1'-N1	5.00	112.20	108.20
1	X	2298	U	C2-N1-C1'	5.00	123.70	117.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1288	A	Sidechain
1	X	1684	G	Sidechain
1	X	219	G	Sidechain
1	X	474	G	Sidechain
1	X	683	A	Sidechain
1	X	739	G	Sidechain

5.2 Too-close contacts (i)

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	431	0
2	Y	2598	0	1328	17	0
3	A	1826	0	1885	62	0
4	B	1539	0	1600	62	0
5	C	1506	0	1525	57	0
6	D	1400	0	1481	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	1286	0	1336	9	0
8	F	503	0	520	3	0
9	G	1114	0	1144	63	0
10	H	997	0	1046	24	0
11	I	1067	0	1103	48	0
12	J	1090	0	1125	32	0
13	K	878	0	930	28	0
14	L	779	0	820	17	0
15	M	871	0	894	29	0
16	N	978	0	1020	25	0
17	O	741	0	756	30	0
18	P	1014	0	1096	20	0
19	Q	726	0	753	23	0
20	R	825	0	881	28	0
21	S	1345	0	1372	21	0
22	T	625	0	655	11	0
23	U	552	0	604	28	0
24	V	533	0	558	4	0
25	W	424	0	470	9	0
26	Z	457	0	462	16	0
27	1	53	0	0	0	0
28	2	46	0	0	2	0
29	3	63	0	0	2	0
30	4	297	0	330	5	0
31	X	30	0	0	0	0
31	Y	5	0	0	0	0
32	X	60	0	66	2	0
All	All	83879	0	54809	969	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 7.

All (969) 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)
13:K:52:ILE:CD1	13:K:52:ILE:CG1	1.93	1.47
11:I:62:LYS:NZ	11:I:64:GLY:HA2	1.60	1.15
1:X:1333:G:N2	1:X:1344:C:H41	1.44	1.12
15:M:79:ARG:HH11	15:M:79:ARG:HG3	1.03	1.10
19:Q:29:VAL:HG11	19:Q:38:ILE:HD11	1.35	1.09
1:X:759:C:H6	1:X:759:C:H5"	1.07	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:542:A:C2	1:X:2004:U:H2'	1.93	1.03
11:I:62:LYS:HZ1	11:I:64:GLY:HA2	1.24	1.02
1:X:542:A:H2	1:X:2004:U:H2'	1.24	1.00
4:B:152:LYS:HB2	9:G:106:TYR:HB3	1.39	1.00
1:X:759:C:H5"	1:X:759:C:C6	1.98	0.98
1:X:617:U:H5	1:X:632:A:C2	1.82	0.96
1:X:1919:A:H2	1:X:1926:U:H3	0.99	0.95
1:X:1333:G:H22	1:X:1344:C:N4	1.62	0.95
1:X:1448:A:H61	1:X:1574:A:H61	0.97	0.94
1:X:1466:C:H2'	1:X:1467:U:O4'	1.69	0.91
16:N:93:LYS:HE3	17:O:5:ILE:HD13	1.52	0.91
1:X:2042:A:H5"	5:C:65:GLY:HA2	1.53	0.91
1:X:1333:G:H22	1:X:1344:C:H41	0.94	0.91
1:X:2371:A:H2	1:X:2403:C:H42	1.15	0.91
15:M:79:ARG:HG3	15:M:79:ARG:NH1	1.80	0.91
1:X:787:A:H2	1:X:800:U:HO2'	1.16	0.90
9:G:33:ILE:HB	9:G:34:PRO:HD3	1.53	0.89
1:X:617:U:H5	1:X:632:A:H2	1.16	0.89
1:X:1277:G:OP1	26:Z:19:ARG:NH2	2.04	0.89
17:O:5:ILE:HD12	17:O:6:GLN:H	1.35	0.88
1:X:1468:A:H5'	1:X:1472:C:N4	1.87	0.88
1:X:1919:A:H2	1:X:1926:U:N3	1.70	0.88
1:X:1542:G:H22	1:X:1562:G:H1	1.15	0.88
1:X:1770:U:H5	1:X:1775:A:N7	1.73	0.87
26:Z:4:HIS:HB3	26:Z:5:PRO:HD3	1.56	0.86
1:X:617:U:C5	1:X:632:A:C2	2.64	0.86
4:B:152:LYS:CB	9:G:106:TYR:HB3	2.07	0.85
9:G:67:ARG:HG2	9:G:70:PHE:HA	1.56	0.85
1:X:542:A:H2	1:X:2004:U:C2'	1.88	0.85
5:C:43:ALA:HB1	5:C:86:PRO:HB2	1.59	0.83
23:U:48:LYS:HG2	23:U:49:LYS:H	1.42	0.82
1:X:1882:G:N2	1:X:1885:C:H41	1.77	0.82
4:B:131:SER:O	4:B:132:LYS:HG3	1.78	0.81
4:B:54:LYS:HB2	4:B:75:THR:O	1.81	0.81
1:X:971:A:H61	12:J:83:ARG:HH22	1.27	0.81
1:X:1266:G:N7	11:I:32:ARG:NH1	2.29	0.81
1:X:1811:A:H4'	1:X:1812:U:H5"	1.62	0.80
11:I:62:LYS:HZ3	11:I:64:GLY:HA2	1.45	0.80
1:X:1173:G:H21	17:O:88:GLN:HE22	1.29	0.80
9:G:132:PHE:CZ	9:G:145:HIS:HB2	2.16	0.80
1:X:70:A:H5'	1:X:71:A:H3'	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.63	0.79
11:I:58:ALA:O	11:I:59:ARG:HB2	1.80	0.79
1:X:689:A:H8	1:X:2052:G:H21	1.31	0.79
1:X:482:A:H2'	1:X:483:A:O4'	1.83	0.78
1:X:320:A:N3	1:X:340:G:O2'	2.15	0.78
9:G:33:ILE:HB	9:G:34:PRO:CD	2.13	0.78
1:X:215:G:H21	1:X:632:A:H8	1.33	0.77
23:U:22:GLY:HA3	23:U:39:LYS:HD2	1.66	0.77
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.99	0.77
19:Q:61:LYS:H	19:Q:72:ARG:HA	1.50	0.77
1:X:1448:A:N6	1:X:1574:A:H61	1.79	0.76
1:X:1673:C:H5"	4:B:136:ARG:CD	2.15	0.76
1:X:1333:G:N2	1:X:1344:C:N4	2.25	0.76
1:X:463:C:H42	1:X:467:U:H5	1.30	0.76
4:B:116:VAL:HG22	4:B:136:ARG:HE	1.50	0.76
1:X:1963:G:O2'	1:X:1965:U:OP2	2.03	0.76
4:B:50:GLY:HA3	4:B:75:THR:HG21	1.67	0.75
16:N:66:ASN:ND2	16:N:70:ARG:HH12	1.84	0.75
15:M:79:ARG:HH11	15:M:79:ARG:CG	1.92	0.75
5:C:48:ARG:HB2	5:C:51:VAL:HG22	1.69	0.75
1:X:2617:G:P	4:B:82:ARG:HH22	2.10	0.74
13:K:17:ARG:NH1	13:K:20:LEU:HD23	2.01	0.74
2:Y:46:G:H5'	6:D:92:ARG:HH12	1.53	0.74
1:X:2551:A:N7	4:B:145:LYS:HB2	2.04	0.73
1:X:1054:C:H42	1:X:1123:G:H1	1.37	0.73
17:O:10:LYS:HG3	17:O:11:GLN:HG2	1.70	0.72
1:X:1811:A:H5"	3:A:161:THR:HG21	1.71	0.72
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.71	0.72
3:A:231:HIS:HD2	3:A:233:HIS:H	1.35	0.72
1:X:1673:C:C5'	4:B:136:ARG:HD2	2.19	0.71
1:X:2042:A:H5"	5:C:65:GLY:CA	2.19	0.71
1:X:759:C:C5'	1:X:759:C:H6	1.95	0.71
1:X:2266:A:H2	1:X:2325:A:H62	1.38	0.71
25:W:12:ARG:CG	25:W:12:ARG:HH11	2.02	0.71
25:W:12:ARG:HG2	25:W:12:ARG:HH11	1.56	0.71
3:A:231:HIS:CD2	3:A:233:HIS:H	2.08	0.71
1:X:1675:C:OP1	4:B:134:TRP:NE1	2.24	0.71
1:X:2653:A:O2'	10:H:41:ASN:ND2	2.24	0.71
4:B:116:VAL:HG22	4:B:136:ARG:NE	2.05	0.70
1:X:304:A:H2'	1:X:305:A:H5"	1.71	0.70
18:P:92:VAL:HG13	18:P:126:ILE:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:17:SER:HB2	23:U:44:ALA:HA	1.74	0.70
23:U:48:LYS:CG	23:U:49:LYS:H	2.04	0.70
13:K:79:VAL:HA	13:K:83:VAL:HG13	1.74	0.70
1:X:1030:U:H3	1:X:1153:A:H62	1.38	0.70
1:X:640:C:H4'	1:X:660:G:H21	1.54	0.70
1:X:2772:U:H3	1:X:2780:A:H61	1.39	0.70
5:C:38:ARG:HH12	5:C:176:ASN:HD21	1.40	0.69
4:B:16:LYS:HB2	4:B:21:ILE:HD11	1.73	0.69
3:A:36:ALA:HB1	3:A:62:TYR:O	1.91	0.69
9:G:100:TYR:HB2	9:G:116:ARG:HH11	1.58	0.69
1:X:1673:C:H5"	4:B:136:ARG:HD2	1.75	0.69
17:O:66:GLY:O	17:O:87:ARG:NH1	2.26	0.69
23:U:32:ARG:HE	23:U:32:ARG:H	1.41	0.69
1:X:2779:C:H2'	1:X:2780:A:C8	2.28	0.69
4:B:7:THR:HG21	15:M:5:ILE:HD11	1.75	0.68
1:X:415:A:H61	1:X:436:A:H61	1.41	0.68
1:X:797:A:C5	3:A:229:VAL:HG21	2.28	0.68
13:K:11:ASN:OD1	13:K:11:ASN:N	2.26	0.68
1:X:1753:A:O5'	1:X:1753:A:H8	1.76	0.68
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.47	0.68
1:X:1238:A:H4'	17:O:83:ARG:HG2	1.76	0.68
15:M:34:ARG:NH2	15:M:88:VAL:HG13	2.09	0.68
1:X:797:A:N7	3:A:229:VAL:HG21	2.08	0.67
15:M:27:PHE:HA	15:M:96:ARG:HH21	1.59	0.67
1:X:2501:U:H5"	1:X:2501:U:H6	1.59	0.67
10:H:98:ILE:HG22	10:H:106:ARG:HG3	1.76	0.67
11:I:76:LYS:HB2	11:I:79:GLN:HG2	1.76	0.67
16:N:83:LEU:HD12	16:N:113:SER:HB2	1.77	0.67
16:N:88:ILE:HG13	17:O:49:GLU:HB2	1.76	0.67
23:U:47:HIS:CD2	23:U:48:LYS:H	2.13	0.66
1:X:841:G:H2'	1:X:842:A:C8	2.30	0.66
23:U:48:LYS:HG2	23:U:49:LYS:N	2.10	0.66
1:X:38:G:H1	1:X:453:U:H3	1.43	0.66
1:X:652:C:H42	1:X:657:A:H61	1.42	0.66
1:X:1586:A:H5'	3:A:38:PRO:HG3	1.76	0.66
1:X:1816:G:O2'	3:A:252:LYS:HG2	1.95	0.66
1:X:1468:A:H5'	1:X:1472:C:H41	1.56	0.66
3:A:89:SER:HB2	3:A:201:HIS:CE1	2.30	0.66
12:J:14:PHE:HE1	12:J:90:ALA:HA	1.59	0.65
1:X:219:G:N2	1:X:231:G:H2'	2.12	0.65
1:X:1467:U:H2'	1:X:1468:A:OP1	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:4:HIS:HB3	26:Z:5:PRO:CD	2.24	0.65
9:G:70:PHE:CB	16:N:64:ARG:HG2	2.27	0.65
1:X:1770:U:C5	1:X:1775:A:N7	2.61	0.65
1:X:2266:A:H62	1:X:2323:U:H3	1.43	0.65
6:D:80:ARG:HD3	6:D:83:MET:HB2	1.78	0.65
1:X:1466:C:C2'	1:X:1467:U:O4'	2.44	0.65
11:I:28:LYS:HE3	11:I:36:GLY:HA3	1.79	0.65
12:J:40:PRO:HB3	12:J:99:LYS:HD2	1.78	0.65
19:Q:60:GLY:H	19:Q:72:ARG:HD3	1.62	0.64
20:R:92:THR:HB	20:R:95:ARG:HH22	1.60	0.64
3:A:183:ARG:HH11	3:A:183:ARG:HB3	1.62	0.64
2:Y:45:C:H2'	6:D:92:ARG:NH1	2.12	0.64
23:U:22:GLY:HA3	23:U:39:LYS:CD	2.27	0.64
3:A:96:HIS:HE1	3:A:100:GLY:HA2	1.62	0.64
11:I:30:ALA:HB3	11:I:34:HIS:CE1	2.32	0.64
1:X:1584:G:H4'	3:A:59:LYS:HB3	1.80	0.64
1:X:2222:U:H2'	1:X:2223:U:C6	2.32	0.64
3:A:172:TYR:HA	3:A:186:HIS:HA	1.80	0.64
20:R:105:ARG:HH12	20:R:112:LYS:HA	1.63	0.63
1:X:1033:G:N2	1:X:1153:A:C2	2.66	0.63
13:K:17:ARG:HH11	13:K:20:LEU:HD23	1.60	0.63
9:G:61:ARG:HH11	9:G:66:HIS:H	1.44	0.63
1:X:2545:A:H61	10:H:40:GLY:HA3	1.63	0.63
1:X:1673:C:H5"	4:B:136:ARG:HD3	1.79	0.63
11:I:28:LYS:HZ1	11:I:37:GLN:H	1.47	0.63
9:G:70:PHE:HB3	16:N:64:ARG:HG2	1.81	0.63
1:X:1803:G:H21	3:A:46:ARG:HD2	1.64	0.63
15:M:25:PRO:HD2	15:M:91:VAL:HG12	1.81	0.63
1:X:203:G:H1'	1:X:205:A:H61	1.64	0.63
5:C:133:PHE:HB2	5:C:160:ALA:HB1	1.81	0.62
9:G:161:GLN:HG2	9:G:165:VAL:HG11	1.80	0.62
3:A:244:ARG:HB3	3:A:252:LYS:NZ	2.13	0.62
4:B:55:ALA:HB3	4:B:58:LYS:HG3	1.81	0.62
1:X:564:U:H2'	1:X:565:A:C8	2.33	0.62
11:I:73:GLU:OE1	11:I:101:ARG:HB2	1.98	0.62
1:X:2790:C:O2'	26:Z:43:HIS:HD2	1.82	0.62
16:N:66:ASN:HB3	16:N:76:TYR:H	1.64	0.62
1:X:1007:A:H4'	16:N:93:LYS:HB3	1.81	0.62
13:K:24:GLN:HB3	13:K:44:LEU:HD22	1.82	0.62
20:R:22:VAL:HG11	20:R:80:LYS:HZ3	1.64	0.62
1:X:82:G:H1	1:X:100:G:H2'	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1033:G:H4'	1:X:1034:U:H5'	1.82	0.62
32:X:2931:1F3:H61	32:X:2931:1F3:H20	1.81	0.61
11:I:32:ARG:HD2	17:O:79:GLN:NE2	2.15	0.61
20:R:46:VAL:HG11	20:R:80:LYS:HD3	1.81	0.61
1:X:617:U:C5	1:X:632:A:H2	2.06	0.61
20:R:92:THR:HB	20:R:95:ARG:NH2	2.16	0.61
5:C:164:VAL:C	5:C:166:TRP:H	2.04	0.61
1:X:346:C:H2'	1:X:347:C:C6	2.36	0.61
1:X:2037:A:H2'	26:Z:8:LYS:HE3	1.82	0.60
1:X:224:G:OP2	1:X:226:C:N4	2.31	0.60
1:X:971:A:N6	12:J:83:ARG:HH22	1.99	0.60
1:X:774:A:H8	1:X:774:A:O5'	1.85	0.60
4:B:116:VAL:H	4:B:136:ARG:HE	1.49	0.60
1:X:2197:U:H2'	1:X:2198:U:C6	2.37	0.60
1:X:649:G:H1	1:X:660:G:H1	1.49	0.60
1:X:540:G:O6	1:X:2006:G:OP1	2.18	0.60
10:H:85:ASP:HB3	15:M:87:LEU:HD12	1.83	0.60
9:G:62:ILE:HG22	9:G:135:LEU:HD21	1.84	0.60
9:G:67:ARG:CG	9:G:70:PHE:HA	2.29	0.60
13:K:11:ASN:OD1	13:K:17:ARG:NH2	2.33	0.60
16:N:66:ASN:HD22	16:N:70:ARG:HH12	1.49	0.60
17:O:5:ILE:HD12	17:O:6:GLN:N	2.12	0.60
1:X:2334:C:H1'	22:T:39:ARG:HH21	1.65	0.60
1:X:2551:A:C8	4:B:144:ARG:HD3	2.37	0.60
1:X:946:U:H2'	1:X:947:C:H6	1.67	0.59
17:O:11:GLN:HE22	17:O:38:LEU:HB3	1.65	0.59
1:X:2362:G:H2'	1:X:2363:G:C8	2.37	0.59
16:N:66:ASN:HB3	16:N:76:TYR:N	2.18	0.59
1:X:2597:G:H21	4:B:150:VAL:HG11	1.66	0.59
5:C:3:GLN:HG2	5:C:116:LYS:HD2	1.84	0.59
20:R:10:HIS:O	20:R:11:ASN:HB2	2.02	0.59
1:X:504:G:H21	18:P:78:ASN:HD21	1.51	0.59
1:X:2713:A:H61	4:B:203:LYS:HG2	1.68	0.59
1:X:760:U:C6	26:Z:3:LYS:HG3	2.38	0.59
4:B:152:LYS:HD2	9:G:106:TYR:H	1.68	0.59
1:X:512:A:H4'	18:P:15:LYS:HB3	1.84	0.59
12:J:92:GLU:HG3	12:J:93:TYR:HD2	1.67	0.58
1:X:827:C:H2'	1:X:828:C:H6	1.68	0.58
25:W:4:LYS:HG2	25:W:52:GLU:HB3	1.85	0.58
1:X:597:U:O4	1:X:683:A:H1'	2.03	0.58
1:X:946:U:H2'	1:X:947:C:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:78:SER:HA	10:H:91:PHE:O	2.04	0.58
29:3:10:ALA:CA	29:3:12:ARG:CA	2.82	0.58
11:I:81:GLN:HG2	11:I:114:ILE:HG22	1.86	0.58
18:P:13:GLN:O	18:P:16:GLN:HG2	2.02	0.58
1:X:2371:A:H8	11:I:59:ARG:HG3	1.69	0.58
1:X:1050:G:H1	1:X:1127:C:H42	1.51	0.58
1:X:2617:G:P	4:B:82:ARG:NH2	2.76	0.58
3:A:91:ARG:HG3	3:A:198:ASN:H	1.69	0.58
9:G:61:ARG:NH1	9:G:66:HIS:H	2.02	0.58
1:X:1468:A:H5'	1:X:1472:C:H42	1.68	0.58
1:X:451:A:H2'	1:X:452:G:C8	2.39	0.58
3:A:39:LYS:HB2	3:A:62:TYR:HB2	1.86	0.58
4:B:120:TRP:HB3	4:B:155:ARG:HH11	1.69	0.58
20:R:16:PHE:HZ	20:R:46:VAL:HG22	1.69	0.58
5:C:48:ARG:C	5:C:50:GLN:H	2.07	0.57
5:C:43:ALA:CB	5:C:86:PRO:HB2	2.32	0.57
1:X:1962:C:H2'	1:X:1963:G:H5'	1.85	0.57
1:X:1773:C:H1'	1:X:2588:U:H5"	1.85	0.57
1:X:623:G:H3'	1:X:624:A:H5"	1.86	0.57
5:C:27:LEU:O	5:C:31:VAL:HG23	2.05	0.57
15:M:32:THR:CG2	15:M:91:VAL:HG22	2.34	0.57
18:P:40:LEU:HB3	26:Z:25:LEU:HD13	1.86	0.57
12:J:99:LYS:HG3	12:J:100:PRO:HD2	1.87	0.57
1:X:1287:A:H2'	1:X:1288:A:H5"	1.86	0.57
1:X:759:C:C5'	1:X:759:C:C6	2.78	0.57
9:G:102:ARG:HB3	9:G:102:ARG:HH11	1.70	0.57
11:I:17:LYS:O	11:I:18:ARG:HB2	2.03	0.57
16:N:88:ILE:HG23	17:O:48:GLY:HA3	1.86	0.57
1:X:1918:G:H1'	1:X:1947:G:N2	2.20	0.57
4:B:131:SER:O	4:B:132:LYS:CG	2.52	0.57
1:X:1811:A:H4'	1:X:1812:U:C5'	2.32	0.57
1:X:787:A:H2	1:X:800:U:O2'	1.84	0.57
1:X:558:G:O3'	1:X:559:C:H4'	2.03	0.57
1:X:504:G:H4'	18:P:27:VAL:HG13	1.87	0.57
18:P:105:ARG:HD3	18:P:119:LYS:HE3	1.86	0.57
1:X:1882:G:H22	1:X:1885:C:H41	1.49	0.57
9:G:69:ASP:H	9:G:76:GLN:HE21	1.51	0.56
13:K:10:LEU:HA	13:K:17:ARG:HG2	1.86	0.56
4:B:16:LYS:HB2	4:B:21:ILE:CD1	2.35	0.56
2:Y:45:C:H2'	6:D:92:ARG:HH11	1.69	0.56
1:X:954:U:OP2	11:I:38:LYS:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:670:U:H2'	1:X:671:A:C8	2.40	0.56
13:K:3:HIS:CG	13:K:5:LYS:HZ3	2.23	0.56
15:M:31:ASP:N	15:M:31:ASP:OD2	2.31	0.56
1:X:673:G:H5'	5:C:93:TYR:CD1	2.41	0.56
6:D:47:SER:HA	6:D:50:ILE:HD12	1.87	0.56
1:X:1030:U:HO2'	1:X:1032:A:H2	1.52	0.56
17:O:36:LYS:HZ1	17:O:54:TYR:HB3	1.70	0.56
1:X:1033:G:H22	1:X:1153:A:H2	1.49	0.56
9:G:105:GLY:O	9:G:106:TYR:C	2.42	0.56
17:O:10:LYS:HD2	17:O:37:ALA:HB3	1.88	0.56
1:X:1113:C:H2'	1:X:1114:A:H8	1.70	0.56
5:C:176:ASN:HD22	5:C:179:ASP:H	1.54	0.56
5:C:48:ARG:C	5:C:50:GLN:N	2.58	0.56
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.87	0.56
1:X:760:U:O2	1:X:1997:A:H1'	2.06	0.56
11:I:32:ARG:HD2	17:O:79:GLN:HE22	1.70	0.56
1:X:172:A:H61	1:X:175:C:H3'	1.71	0.56
1:X:334:G:H3'	5:C:162:ARG:HE	1.70	0.56
5:C:30:VAL:HG11	5:C:177:VAL:HG21	1.88	0.55
21:S:149:ALA:HA	21:S:152:ILE:HD12	1.87	0.55
4:B:134:TRP:H	4:B:134:TRP:HD1	1.53	0.55
9:G:116:ARG:HD2	9:G:119:LEU:HD12	1.89	0.55
11:I:75:VAL:HG22	11:I:99:VAL:HG11	1.88	0.55
13:K:87:TYR:HE1	13:K:94:TYR:HD2	1.54	0.55
5:C:95:LEU:HD23	5:C:96:PRO:HD2	1.88	0.55
1:X:1032:A:H8	1:X:1033:G:H5"	1.71	0.55
11:I:94:GLU:HA	11:I:97:ARG:HE	1.71	0.55
13:K:33:ARG:HD3	13:K:112:LEU:HD22	1.89	0.55
13:K:7:GLY:O	13:K:8:ARG:HG2	2.06	0.55
20:R:90:LYS:HB2	20:R:108:VAL:HG11	1.88	0.55
23:U:48:LYS:CG	23:U:49:LYS:N	2.70	0.55
1:X:1673:C:H5'	4:B:136:ARG:HD2	1.88	0.55
7:E:164:PHE:HB2	7:E:167:GLU:HB2	1.88	0.55
1:X:1278:A:H2	1:X:1997:A:H62	1.54	0.55
1:X:2387:U:H2'	1:X:2388:G:H8	1.71	0.55
3:A:218:LYS:HE3	3:A:221:GLN:HB2	1.89	0.55
12:J:44:LYS:HD3	12:J:47:GLN:HE22	1.71	0.55
1:X:1373:G:H22	1:X:2192:U:H3	1.54	0.55
1:X:1448:A:H61	1:X:1574:A:N6	1.82	0.55
18:P:14:ARG:HA	18:P:17:GLN:HG2	1.88	0.54
1:X:746:G:N7	1:X:774:A:C6	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:89:SER:HB2	3:A:201:HIS:HE1	1.72	0.54
3:A:96:HIS:HE1	3:A:100:GLY:CA	2.20	0.54
9:G:104:THR:OG1	9:G:110:LEU:HB3	2.07	0.54
19:Q:38:ILE:O	19:Q:42:ILE:HG22	2.07	0.54
21:S:25:ASN:HB3	21:S:85:MET:HB2	1.88	0.54
1:X:1473:U:H6	1:X:1473:U:OP2	1.90	0.54
1:X:2797:G:OP2	13:K:3:HIS:NE2	2.40	0.54
1:X:2617:G:OP2	4:B:82:ARG:NH2	2.40	0.54
12:J:109:GLY:HA3	21:S:112:LEU:HD21	1.90	0.54
18:P:57:LEU:HA	18:P:60:ILE:HD12	1.89	0.54
12:J:12:LYS:O	12:J:13:GLN:HB2	2.08	0.54
2:Y:62:C:H2'	2:Y:63:A:C8	2.42	0.54
16:N:81:ASN:HD22	16:N:117:ARG:HH21	1.56	0.54
5:C:146:GLU:HG3	5:C:185:ARG:HH11	1.72	0.54
1:X:1790:G:H5'	1:X:1811:A:H61	1.73	0.54
11:I:10:PRO:HA	11:I:14:LYS:HB2	1.89	0.54
1:X:2371:A:C8	11:I:59:ARG:HG3	2.41	0.54
1:X:1810:U:H2'	3:A:157:ARG:HD3	1.90	0.54
4:B:147:PRO:C	4:B:149:ARG:H	2.11	0.53
6:D:92:ARG:HB2	6:D:92:ARG:HH21	1.72	0.53
13:K:3:HIS:HB3	13:K:5:LYS:CE	2.39	0.53
1:X:2790:C:O2'	26:Z:43:HIS:CD2	2.61	0.53
11:I:117:ALA:HA	11:I:137:GLY:O	2.08	0.53
18:P:57:LEU:HD13	18:P:69:ALA:HA	1.91	0.53
1:X:346:C:H2'	1:X:347:C:H6	1.73	0.53
10:H:116:ARG:HG3	15:M:38:LYS:HZ3	1.73	0.53
25:W:1:MET:HB3	25:W:34:VAL:HG12	1.90	0.53
1:X:2196:U:H2'	1:X:2197:U:O4'	2.08	0.53
1:X:748:A:H3'	1:X:749:C:H6	1.73	0.53
2:Y:42:U:H1'	2:Y:47:A:H61	1.73	0.53
5:C:98:GLN:HA	5:C:101:GLN:HG3	1.90	0.53
10:H:116:ARG:HG3	15:M:38:LYS:NZ	2.22	0.53
15:M:28:ARG:H	15:M:96:ARG:NH2	2.06	0.53
1:X:1976:U:H4'	4:B:128:SER:OG	2.08	0.53
2:Y:9:G:O2'	14:L:41:GLN:NE2	2.41	0.53
1:X:2306:A:H2'	1:X:2307:A:C8	2.43	0.53
6:D:75:SER:HB2	6:D:79:LEU:HD13	1.90	0.53
9:G:158:HIS:HA	9:G:161:GLN:CD	2.29	0.53
1:X:1467:U:H3'	1:X:1467:U:H6	1.74	0.53
3:A:206:LEU:HA	3:A:211:ARG:HG2	1.90	0.53
23:U:49:LYS:HB2	23:U:61:TRP:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:77:C:H42	1:X:106:G:H1	1.55	0.53
1:X:490:A:N3	1:X:492:G:H5"	2.24	0.53
5:C:148:VAL:HG13	5:C:185:ARG:HB2	1.91	0.53
1:X:2766:U:OP1	4:B:69:LYS:HE2	2.09	0.53
2:Y:83:C:N4	2:Y:98:C:N3	2.57	0.53
6:D:38:GLU:HB3	6:D:87:ILE:HB	1.91	0.53
7:E:89:LEU:HD23	7:E:162:VAL:HG22	1.91	0.53
4:B:149:ARG:CZ	9:G:106:TYR:HD1	2.22	0.53
9:G:61:ARG:HH11	9:G:65:LYS:HB3	1.73	0.53
9:G:67:ARG:NE	9:G:70:PHE:O	2.40	0.53
15:M:27:PHE:HB3	15:M:93:ILE:HD12	1.89	0.53
1:X:172:A:H5"	1:X:173:A:OP2	2.09	0.53
5:C:14:THR:HG22	5:C:15:ILE:H	1.74	0.52
13:K:32:GLY:HA2	13:K:115:LEU:HD12	1.91	0.52
20:R:22:VAL:HG11	20:R:80:LYS:HD2	1.91	0.52
1:X:870:C:H4'	22:T:23:VAL:HG21	1.90	0.52
1:X:1519:G:H2'	1:X:1520:G:H8	1.73	0.52
1:X:1943:A:H5"	1:X:1943:A:H8	1.74	0.52
1:X:2272:A:H5"	14:L:15:ARG:HH21	1.73	0.52
1:X:2811:G:H2'	1:X:2812:A:C8	2.45	0.52
3:A:145:LEU:HD23	3:A:155:LEU:HD12	1.92	0.52
1:X:2659:C:H5'	4:B:189:PRO:HA	1.91	0.52
9:G:103:TYR:CE2	9:G:111:LYS:HB2	2.44	0.52
9:G:67:ARG:HB3	9:G:70:PHE:HA	1.90	0.52
1:X:2241:U:H5	22:T:17:ASN:OD1	1.92	0.52
1:X:823:U:OP1	11:I:32:ARG:NH1	2.42	0.52
1:X:793:G:H21	1:X:796:A:H62	1.57	0.52
20:R:16:PHE:CE2	20:R:80:LYS:HE2	2.43	0.52
1:X:2505:G:H1'	30:4:1:MET:HB2	1.91	0.52
10:H:41:ASN:H	10:H:41:ASN:ND2	2.07	0.52
9:G:68:PRO:HD2	9:G:76:GLN:HB3	1.92	0.52
12:J:62:GLY:H	21:S:175:ARG:H	1.57	0.52
21:S:3:LEU:HD11	21:S:33:ALA:H	1.75	0.52
19:Q:66:GLY:C	19:Q:68:PHE:H	2.13	0.52
1:X:2484:G:C2	32:X:2931:1F3:H7	2.45	0.52
19:Q:68:PHE:O	19:Q:70:GLY:N	2.42	0.52
20:R:60:PRO:HD2	20:R:62:MET:HB2	1.91	0.52
21:S:3:LEU:HD22	21:S:34:LEU:HB3	1.92	0.52
3:A:226:MET:HG2	3:A:230:ASP:HB2	1.92	0.52
1:X:666:U:O2'	1:X:667:U:H5"	2.10	0.52
1:X:760:U:C5	26:Z:3:LYS:HG3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1850:G:H1'	1:X:1867:A:N6	2.25	0.52
1:X:1909:U:H5'	1:X:1911:A:OP2	2.09	0.52
1:X:553:C:H42	1:X:559:C:N4	2.08	0.52
3:A:108:PRO:HB3	3:A:143:HIS:CE1	2.45	0.51
11:I:97:ARG:O	11:I:98:LEU:HB2	2.10	0.51
23:U:41:VAL:HG23	23:U:42:GLN:H	1.74	0.51
12:J:79:PRO:HD2	12:J:88:LYS:HD2	1.90	0.51
15:M:34:ARG:HB2	15:M:91:VAL:HG23	1.91	0.51
11:I:28:LYS:CE	11:I:36:GLY:HA3	2.40	0.51
1:X:2387:U:H2'	1:X:2388:G:C8	2.46	0.51
26:Z:16:ARG:HD3	26:Z:20:ARG:CZ	2.40	0.51
1:X:1805:G:H1'	3:A:50:THR:HG21	1.92	0.51
1:X:1673:C:C5'	4:B:136:ARG:CD	2.80	0.51
23:U:49:LYS:HB3	23:U:61:TRP:CE3	2.46	0.51
1:X:1071:U:H4'	1:X:1072:U:H3'	1.92	0.51
3:A:244:ARG:HB3	3:A:252:LYS:HZ1	1.76	0.51
4:B:46:ALA:HB2	4:B:82:ARG:HG2	1.92	0.51
4:B:110:GLY:O	13:K:3:HIS:CD2	2.64	0.51
19:Q:31:PRO:HA	19:Q:76:LYS:HD2	1.92	0.51
7:E:6:LYS:HB3	7:E:69:ARG:HD2	1.92	0.51
19:Q:12:ILE:HG12	19:Q:13:SER:H	1.74	0.51
1:X:168:A:H2'	1:X:169:C:C6	2.45	0.51
11:I:108:LEU:HD23	11:I:129:ALA:HB1	1.93	0.51
14:L:76:ALA:HB2	14:L:107:ALA:HA	1.91	0.51
1:X:2867:G:O5'	1:X:2867:G:H8	1.93	0.51
9:G:100:TYR:CB	9:G:116:ARG:NH1	2.72	0.51
13:K:45:ARG:HB3	13:K:46:PRO:HD3	1.91	0.51
1:X:2725:C:H1'	7:E:143:GLN:HG3	1.91	0.51
1:X:686:C:H5"	5:C:74:VAL:HB	1.93	0.51
1:X:1685:A:H5"	10:H:5:GLN:HG2	1.92	0.50
17:O:57:GLN:H	17:O:97:GLY:CA	2.25	0.50
21:S:3:LEU:HD21	21:S:32:PHE:HB3	1.93	0.50
1:X:1134:C:H2'	1:X:1135:C:H6	1.76	0.50
12:J:78:LYS:HA	12:J:88:LYS:NZ	2.26	0.50
24:V:23:LYS:O	24:V:27:GLU:HG2	2.10	0.50
1:X:553:C:H42	1:X:559:C:H42	1.58	0.50
13:K:49:GLU:O	13:K:52:ILE:HG12	2.12	0.50
1:X:2406:C:H5"	1:X:2408:G:OP1	2.11	0.50
1:X:2542:U:O2	1:X:2544:A:H8	1.95	0.50
9:G:103:TYR:CG	9:G:111:LYS:HA	2.46	0.50
1:X:1142:G:H5"	9:G:111:LYS:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2355:A:H61	14:L:91:ARG:CZ	2.25	0.50
1:X:2543:A:H5'	1:X:2627:G:H4'	1.93	0.50
3:A:79:VAL:HG21	3:A:111:LEU:HD22	1.94	0.50
13:K:10:LEU:CD2	13:K:17:ARG:HB2	2.42	0.50
17:O:88:GLN:HE21	17:O:88:GLN:HA	1.76	0.50
1:X:1699:A:H61	1:X:1723:U:H3	1.58	0.50
4:B:116:VAL:HG13	4:B:136:ARG:HH21	1.75	0.50
5:C:151:VAL:HG11	5:C:175:VAL:HG22	1.93	0.50
5:C:96:PRO:HB2	5:C:99:VAL:HG23	1.93	0.50
10:H:75:VAL:HG12	10:H:118:LEU:HD11	1.94	0.50
1:X:1467:U:C2'	1:X:1468:A:OP1	2.58	0.50
1:X:1827:G:H1'	1:X:1914:U:C2	2.47	0.50
2:Y:62:C:H2'	2:Y:63:A:H8	1.76	0.50
4:B:147:PRO:C	4:B:149:ARG:N	2.65	0.50
9:G:154:GLU:O	9:G:157:PRO:HD2	2.11	0.50
1:X:2006:G:H5'	1:X:2596:C:H4'	1.93	0.50
9:G:104:THR:OG1	9:G:105:GLY:N	2.44	0.50
9:G:103:TYR:CZ	9:G:111:LYS:HB2	2.46	0.50
1:X:1006:C:O2	16:N:61:TRP:HZ2	1.95	0.50
1:X:1032:A:C8	1:X:1033:G:H5"	2.47	0.50
1:X:347:C:H4'	20:R:15:HIS:CD2	2.48	0.49
11:I:108:LEU:HD13	11:I:120:VAL:HG11	1.94	0.49
1:X:2423:G:P	5:C:62:LYS:HD2	2.52	0.49
11:I:77:LEU:HB2	11:I:111:SER:H	1.77	0.49
1:X:1033:G:H5'	9:G:93:LYS:NZ	2.26	0.49
1:X:341:A:H2	1:X:1223:G:H2'	1.77	0.49
6:D:33:LYS:HB3	6:D:92:ARG:HG2	1.94	0.49
12:J:15:ARG:HB3	12:J:73:LYS:HZ2	1.78	0.49
18:P:103:LEU:HB2	18:P:119:LYS:HB2	1.95	0.49
1:X:1805:G:H1'	3:A:50:THR:CG2	2.43	0.49
18:P:49:SER:O	18:P:51:GLN:N	2.45	0.49
1:X:494:A:C8	20:R:56:LYS:HD2	2.48	0.49
1:X:1443:G:H2'	1:X:1444:C:C6	2.47	0.49
1:X:2657:G:H2'	1:X:2658:A:O4'	2.13	0.49
5:C:22:VAL:HG13	5:C:106:MET:HG2	1.93	0.49
9:G:106:TYR:O	9:G:110:LEU:HD12	2.12	0.49
11:I:47:ALA:O	11:I:49:PHE:N	2.41	0.49
16:N:17:VAL:HG11	16:N:36:PHE:HB2	1.94	0.49
17:O:38:LEU:HD23	17:O:47:PHE:HB3	1.95	0.49
1:X:1219:C:H5"	11:I:7:LYS:HE2	1.93	0.49
1:X:2490:U:H2'	1:X:2491:C:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:16:ARG:HD3	26:Z:20:ARG:NH1	2.28	0.49
11:I:62:LYS:HZ3	11:I:64:GLY:CA	2.21	0.49
13:K:3:HIS:CG	13:K:5:LYS:NZ	2.80	0.49
16:N:75:ASN:ND2	16:N:78:THR:H	2.10	0.49
1:X:2178:U:H2'	1:X:2179:C:C6	2.48	0.49
1:X:418:C:H4'	1:X:418:C:OP2	2.13	0.49
1:X:746:G:N7	1:X:774:A:C5	2.81	0.49
3:A:150:GLY:O	3:A:152:GLY:N	2.46	0.49
3:A:161:THR:O	3:A:196:VAL:HG23	2.13	0.49
10:H:83:ARG:NE	10:H:89:ILE:HD11	2.28	0.49
13:K:10:LEU:HD23	13:K:17:ARG:HB2	1.95	0.49
18:P:38:VAL:HG12	18:P:97:VAL:HG21	1.95	0.49
19:Q:71:GLN:HG2	19:Q:72:ARG:N	2.27	0.49
1:X:1674:C:H2'	1:X:1675:C:H6	1.78	0.49
4:B:2:LYS:HB2	4:B:200:SER:HB3	1.95	0.48
5:C:45:THR:HG21	5:C:85:GLY:HA3	1.94	0.48
1:X:969:U:C4	12:J:17:ARG:HB2	2.48	0.48
1:X:827:C:H2'	1:X:828:C:C6	2.48	0.48
14:L:27:LEU:HD23	14:L:44:ASP:HA	1.95	0.48
1:X:2212:U:H2'	1:X:2213:G:C8	2.48	0.48
14:L:68:ALA:HB1	14:L:102:ALA:HB3	1.95	0.48
14:L:8:ARG:HG3	14:L:9:ARG:H	1.77	0.48
16:N:49:ASP:HA	16:N:52:ASN:HB2	1.95	0.48
24:V:25:LEU:HD21	24:V:47:ARG:HG2	1.95	0.48
1:X:224:G:H4'	1:X:399:G:C5	2.48	0.48
1:X:609:U:H5'	11:I:18:ARG:HD3	1.94	0.48
21:S:132:GLN:HE21	21:S:132:GLN:H	1.61	0.48
1:X:1329:U:H2'	1:X:1330:G:C8	2.48	0.48
10:H:110:VAL:HG23	10:H:129:LEU:HD12	1.94	0.48
15:M:5:ILE:HB	15:M:7:ILE:HG12	1.95	0.48
1:X:791:G:H5'	3:A:48:ARG:HH21	1.77	0.48
6:D:123:ASP:HB3	6:D:127:ASN:HB2	1.96	0.48
7:E:9:ILE:HD11	7:E:69:ARG:HG2	1.95	0.48
14:L:30:SER:O	14:L:40:ALA:HA	2.13	0.48
14:L:30:SER:HB2	14:L:43:ILE:HD11	1.96	0.48
1:X:1833:U:H2'	1:X:1834:G:C8	2.48	0.48
1:X:2362:G:H2'	1:X:2363:G:H8	1.77	0.48
1:X:517:A:H5"	1:X:518:A:H5'	1.96	0.48
9:G:96:ASP:O	9:G:98:LYS:N	2.46	0.48
11:I:13:ARG:HE	11:I:13:ARG:H	1.62	0.48
14:L:8:ARG:HG3	14:L:9:ARG:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:70:PHE:HB2	16:N:64:ARG:HG2	1.94	0.48
1:X:2209:G:H4'	23:U:46:LEU:HB2	1.96	0.48
20:R:95:ARG:HH12	20:R:107:ALA:H	1.61	0.48
1:X:1922:U:OP1	1:X:2583:U:O2'	2.29	0.48
1:X:879:A:H2'	1:X:879:A:N3	2.29	0.48
1:X:2307:A:H2'	1:X:2308:A:C8	2.49	0.48
21:S:91:PRO:HG2	21:S:125:PRO:HD2	1.96	0.48
1:X:1753:A:O5'	1:X:1753:A:C8	2.63	0.48
1:X:1777:A:H1'	1:X:1921:A:N6	2.29	0.48
1:X:2522:G:H2'	1:X:2523:G:C8	2.49	0.48
1:X:572:G:N3	16:N:37:GLN:NE2	2.60	0.48
13:K:3:HIS:HB3	13:K:5:LYS:HE2	1.96	0.47
20:R:25:LEU:HD12	20:R:81:VAL:HB	1.96	0.47
1:X:1169:C:H4'	25:W:28:ILE:O	2.14	0.47
1:X:1468:A:H8	1:X:1468:A:O5'	1.97	0.47
1:X:2774:U:O2'	1:X:2775:U:H5"	2.14	0.47
14:L:12:ARG:HA	14:L:92:GLY:O	2.14	0.47
21:S:117:VAL:HB	21:S:168:VAL:HG13	1.97	0.47
1:X:88:G:OP2	1:X:89:A:H3'	2.14	0.47
1:X:1257:U:H5"	11:I:17:LYS:HG3	1.95	0.47
21:S:3:LEU:HD13	21:S:4:THR:H	1.78	0.47
1:X:1582:A:OP1	3:A:211:ARG:NE	2.43	0.47
1:X:1685:A:N6	1:X:1693:A:H61	2.12	0.47
1:X:2516:U:H2'	1:X:2517:C:C6	2.49	0.47
23:U:43:ARG:HG2	23:U:44:ALA:N	2.30	0.47
1:X:1998:A:N3	26:Z:6:VAL:HG23	2.29	0.47
1:X:2779:C:H2'	1:X:2780:A:H8	1.79	0.47
3:A:43:ARG:HH21	3:A:54:ILE:HG13	1.80	0.47
5:C:186:LEU:HG	5:C:188:ILE:HG12	1.95	0.47
9:G:132:PHE:HB2	9:G:145:HIS:CE1	2.49	0.47
17:O:11:GLN:NE2	17:O:38:LEU:HB3	2.30	0.47
5:C:3:GLN:O	5:C:12:GLY:HA3	2.15	0.47
11:I:78:SER:HB3	11:I:112:GLY:HA3	1.96	0.47
1:X:503:G:H2'	1:X:504:G:O4'	2.15	0.47
1:X:681:A:H8	1:X:681:A:H5"	1.79	0.47
20:R:105:ARG:HH22	20:R:112:LYS:CA	2.28	0.47
1:X:1173:G:H1'	17:O:21:ARG:HD2	1.97	0.47
3:A:244:ARG:HB3	3:A:252:LYS:HZ2	1.80	0.47
1:X:2860:C:H2'	1:X:2861:A:O4'	2.14	0.47
2:Y:64:C:H2'	2:Y:65:A:H8	1.79	0.47
13:K:11:ASN:ND2	13:K:12:ARG:HE	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1662:G:H5"	1:X:1663:C:H5'	1.96	0.47
1:X:1787:U:H2'	1:X:1788:C:C6	2.50	0.47
1:X:1854:G:H1	1:X:1863:U:H3	1.62	0.47
1:X:2498:U:H4'	1:X:2499:C:OP1	2.14	0.47
1:X:922:A:H2'	1:X:923:A:C8	2.50	0.47
26:Z:16:ARG:O	26:Z:20:ARG:HD2	2.14	0.47
30:4:2:LYS:HA	30:4:2:LYS:HE2	1.97	0.47
5:C:112:GLN:HA	5:C:116:LYS:HD3	1.96	0.47
17:O:57:GLN:H	17:O:97:GLY:HA2	1.79	0.47
20:R:22:VAL:HG13	20:R:81:VAL:O	2.14	0.47
22:T:14:ARG:HG3	22:T:15:ASP:H	1.80	0.47
1:X:1287:A:C2'	1:X:1288:A:H5"	2.45	0.47
1:X:1342:U:H5"	1:X:1343:C:H5	1.80	0.47
1:X:2343:C:H2'	1:X:2344:G:O4'	2.15	0.47
1:X:203:G:H5'	1:X:234:C:H4'	1.97	0.47
1:X:241:C:H2'	1:X:242:A:H5"	1.96	0.47
9:G:75:ILE:HG13	9:G:75:ILE:H	1.58	0.47
4:B:195:LEU:H	15:M:2:GLN:HG2	1.79	0.46
7:E:17:VAL:HG13	7:E:26:VAL:HG22	1.97	0.46
8:F:77:LEU:HD13	8:F:107:ILE:HG23	1.96	0.46
1:X:1367:A:H2'	1:X:1368:G:O4'	2.16	0.46
1:X:1509:A:H8	1:X:1510:A:C8	2.33	0.46
1:X:1788:C:H2'	1:X:1789:U:H6	1.81	0.46
1:X:341:A:C2	1:X:1223:G:H2'	2.50	0.46
3:A:67:PHE:HD2	3:A:153:ALA:HB3	1.79	0.46
5:C:158:ARG:HA	5:C:169:VAL:HG21	1.96	0.46
12:J:69:ILE:HG23	12:J:104:MET:HA	1.97	0.46
23:U:47:HIS:HD2	23:U:48:LYS:O	1.97	0.46
4:B:120:TRP:O	4:B:121:ASN:HB2	2.14	0.46
20:R:15:HIS:O	20:R:16:PHE:HB3	2.15	0.46
1:X:341:A:HO2'	1:X:342:G:H8	1.63	0.46
3:A:243:GLY:C	3:A:244:ARG:HD3	2.36	0.46
14:L:10:LYS:O	14:L:14:ARG:HB2	2.16	0.46
1:X:1278:A:H61	1:X:1996:A:H5"	1.80	0.46
1:X:2661:G:O6	1:X:2708:U:H1'	2.16	0.46
1:X:651:C:H2'	1:X:652:C:H5"	1.98	0.46
30:4:19:ARG:HB2	30:4:24:LEU:HD13	1.98	0.46
3:A:43:ARG:HD2	3:A:43:ARG:N	2.31	0.46
4:B:131:SER:O	4:B:132:LYS:CB	2.64	0.46
4:B:133:LYS:HE2	4:B:133:LYS:HB3	1.61	0.46
5:C:176:ASN:HB3	5:C:179:ASP:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:124:ALA:HB3	7:E:132:ASP:HB2	1.97	0.46
9:G:108:GLY:H	9:G:110:LEU:HG	1.79	0.46
1:X:240:U:H2'	1:X:241:C:O4'	2.15	0.46
1:X:956:A:C4	1:X:2427:A:C2	3.03	0.46
26:Z:33:CYS:SG	26:Z:46:CYS:SG	3.11	0.46
3:A:252:LYS:H	3:A:252:LYS:HE3	1.80	0.46
5:C:5:ASN:HB2	5:C:10:ASN:HA	1.98	0.46
9:G:36:ASN:O	9:G:38:GLU:N	2.34	0.46
15:M:27:PHE:HB3	15:M:93:ILE:CD1	2.45	0.46
21:S:87:THR:O	21:S:88:TYR:HB3	2.16	0.46
1:X:590:C:H2'	1:X:591:G:C8	2.51	0.46
9:G:90:LEU:HD23	9:G:94:LYS:HA	1.98	0.46
14:L:66:ASP:C	14:L:68:ALA:H	2.19	0.46
16:N:74:MET:HB3	16:N:75:ASN:H	1.63	0.46
1:X:1845:A:N1	1:X:2070:G:H1'	2.30	0.46
1:X:2266:A:N6	1:X:2323:U:H3	2.13	0.46
3:A:67:PHE:HB3	3:A:153:ALA:H	1.81	0.46
9:G:162:LYS:N	9:G:163:PRO:HD2	2.31	0.46
10:H:27:SER:HB2	10:H:121:ARG:HH22	1.81	0.46
10:H:24:VAL:HA	10:H:51:ILE:HG22	1.98	0.46
12:J:73:LYS:HB3	12:J:95:VAL:HG12	1.97	0.46
20:R:25:LEU:H	20:R:80:LYS:HA	1.81	0.46
23:U:10:LYS:HD3	23:U:60:VAL:HG21	1.97	0.46
1:X:1882:G:H21	1:X:1885:C:H41	1.62	0.46
1:X:627:A:H2'	1:X:628:A:C8	2.50	0.46
11:I:57:ILE:HA	11:I:57:ILE:HD13	1.93	0.46
1:X:1630:A:C2	18:P:114:ALA:HB2	2.51	0.46
1:X:2167:A:H2'	1:X:2168:A:H8	1.80	0.46
1:X:331:U:H1'	5:C:162:ARG:NH1	2.31	0.46
30:4:19:ARG:HD2	30:4:24:LEU:HD22	1.98	0.46
11:I:30:ALA:HB3	11:I:34:HIS:HE1	1.78	0.46
4:B:181:LEU:HD11	15:M:12:LEU:HD23	1.98	0.46
21:S:127:PRO:C	21:S:129:ARG:H	2.19	0.46
5:C:119:ALA:H	5:C:189:ASP:HA	1.81	0.45
5:C:45:THR:HB	5:C:86:PRO:O	2.15	0.45
9:G:57:LEU:HD22	9:G:170:PRO:HA	1.98	0.45
12:J:14:PHE:CE1	12:J:90:ALA:HA	2.46	0.45
1:X:2795:A:H4'	13:K:5:LYS:HG2	1.97	0.45
3:A:108:PRO:HB3	3:A:143:HIS:HE1	1.81	0.45
3:A:95:LEU:HD12	3:A:105:ILE:HD13	1.98	0.45
10:H:26:ASN:HD22	10:H:26:ASN:HA	1.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2324:G:N3	1:X:2360:C:H2'	2.32	0.45
1:X:2754:C:H2'	1:X:2755:A:O4'	2.17	0.45
1:X:1142:G:OP1	9:G:107:GLN:HB3	2.16	0.45
1:X:1817:U:O4'	3:A:252:LYS:HD3	2.16	0.45
5:C:164:VAL:HB	5:C:165:SER:H	1.57	0.45
9:G:157:PRO:C	9:G:159:SER:H	2.20	0.45
9:G:67:ARG:CB	9:G:70:PHE:HA	2.47	0.45
12:J:28:VAL:HG21	12:J:135:ARG:HA	1.98	0.45
18:P:94:GLU:HG3	18:P:127:ILE:HB	1.99	0.45
1:X:1466:C:H2'	1:X:1467:U:C1'	2.46	0.45
1:X:2477:C:H5'	1:X:2477:C:H6	1.81	0.45
2:Y:54:U:H4'	2:Y:54:U:OP1	2.17	0.45
5:C:102:LEU:O	5:C:106:MET:HB2	2.17	0.45
6:D:40:LEU:HD21	6:D:87:ILE:HD12	1.98	0.45
11:I:108:LEU:HB2	11:I:122:VAL:HG11	1.98	0.45
4:B:14:ILE:HG13	15:M:20:HIS:CE1	2.52	0.45
19:Q:11:VAL:HB	19:Q:26:SER:HB2	1.99	0.45
1:X:1468:A:O5'	1:X:1468:A:C8	2.70	0.45
1:X:2397:A:H2'	1:X:2398:U:O4'	2.17	0.45
1:X:2772:U:H2'	1:X:2773:G:C8	2.52	0.45
1:X:29:U:H6	1:X:29:U:O5'	2.00	0.45
20:R:48:VAL:HG12	20:R:50:GLY:H	1.80	0.45
1:X:1467:U:C5'	1:X:1467:U:C6	3.00	0.45
1:X:2074:U:H1'	23:U:48:LYS:HE3	1.97	0.45
1:X:227:G:H2'	1:X:228:A:C8	2.52	0.45
1:X:336:A:H2'	1:X:337:G:C8	2.52	0.45
1:X:1268:U:C2	5:C:66:ASN:HA	2.52	0.45
9:G:132:PHE:CE2	9:G:145:HIS:HB2	2.51	0.45
1:X:1187:A:H2'	1:X:1188:A:C8	2.52	0.45
5:C:43:ALA:HB1	5:C:86:PRO:CB	2.41	0.45
6:D:136:LEU:HD11	6:D:143:TYR:HB2	1.99	0.45
8:F:93:LYS:HA	21:S:109:GLN:HG3	1.98	0.45
10:H:2:ILE:HB	10:H:45:ALA:HB3	1.99	0.45
13:K:17:ARG:NH1	13:K:20:LEU:CD2	2.77	0.45
17:O:69:ILE:HG22	17:O:86:HIS:HB3	1.98	0.45
1:X:1218:C:O4'	11:I:13:ARG:HD3	2.16	0.45
1:X:1467:U:H5	1:X:1468:A:O4'	2.00	0.45
3:A:250:TRP:HB3	3:A:251:GLY:H	1.54	0.45
4:B:146:THR:OG1	4:B:147:PRO:HD3	2.17	0.45
5:C:45:THR:HG22	5:C:47:THR:OG1	2.17	0.45
23:U:29:GLY:C	23:U:31:GLY:H	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1373:G:H1	1:X:2192:U:H3	1.64	0.45
1:X:2797:G:OP2	13:K:3:HIS:CD2	2.69	0.45
1:X:231:G:H4'	1:X:397:U:H5"	1.98	0.45
1:X:1467:U:C5	1:X:1468:A:O4'	2.70	0.45
1:X:1919:A:C2	1:X:1926:U:N3	2.62	0.45
25:W:3:ILE:HD12	25:W:51:LEU:HD13	1.99	0.44
1:X:1022:A:H5"	16:N:77:SER:HB2	2.00	0.44
1:X:1234:C:H2'	1:X:1235:C:H6	1.82	0.44
1:X:1437:A:H2'	1:X:1438:G:H8	1.82	0.44
5:C:146:GLU:HG3	5:C:185:ARG:NH1	2.32	0.44
8:F:79:ARG:HG2	8:F:84:ILE:HB	1.99	0.44
3:A:147:LEU:HD22	3:A:183:ARG:HH22	1.81	0.44
1:X:1675:C:OP1	4:B:134:TRP:CD1	2.69	0.44
1:X:814:G:OP1	5:C:50:GLN:HB2	2.18	0.44
10:H:116:ARG:HG3	15:M:38:LYS:CE	2.47	0.44
19:Q:29:VAL:HG21	19:Q:38:ILE:HG13	1.98	0.44
23:U:22:GLY:N	23:U:39:LYS:HB2	2.32	0.44
1:X:424:G:H4'	1:X:425:A:O5'	2.18	0.44
1:X:800:U:H5"	1:X:801:A:H5'	1.99	0.44
9:G:132:PHE:CE1	9:G:145:HIS:HB2	2.52	0.44
15:M:28:ARG:O	15:M:96:ARG:NH2	2.50	0.44
20:R:45:LYS:HA	20:R:76:LEU:O	2.16	0.44
7:E:103:LEU:HD11	7:E:131:ILE:HG12	1.99	0.44
1:X:2545:A:N6	10:H:40:GLY:HA3	2.31	0.44
13:K:3:HIS:CE1	13:K:5:LYS:HZ3	2.34	0.44
12:J:61:ARG:HG2	21:S:175:ARG:HG3	2.00	0.44
3:A:248:THR:HB	3:A:249:PRO:HD2	2.00	0.44
5:C:74:VAL:HG23	5:C:76:THR:H	1.83	0.44
12:J:11:ARG:HH12	12:J:72:ASP:HB2	1.83	0.44
12:J:92:GLU:HG3	12:J:93:TYR:CD2	2.51	0.44
13:K:46:PRO:O	13:K:50:GLN:HG3	2.18	0.44
1:X:1190:C:H2'	1:X:1191:G:H8	1.82	0.44
1:X:341:A:O2'	1:X:342:G:H8	2.01	0.44
1:X:553:C:H4'	1:X:554:U:OP1	2.17	0.44
1:X:1030:U:O2'	1:X:1032:A:H2	1.99	0.44
1:X:689:A:H8	1:X:2052:G:N2	2.06	0.44
28:2:26:SER:CA	28:2:27:GLY:CA	2.95	0.44
1:X:673:G:H5'	5:C:93:TYR:CE1	2.52	0.44
17:O:23:GLU:HB2	17:O:91:THR:HG21	1.99	0.44
17:O:72:ARG:HD2	17:O:83:ARG:HH11	1.82	0.44
19:Q:60:GLY:H	19:Q:72:ARG:HH11	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1012:A:H2'	1:X:1013:G:O4'	2.17	0.44
1:X:1255:A:H2'	1:X:1256:C:C6	2.53	0.44
1:X:585:U:H2'	1:X:586:G:C8	2.52	0.44
1:X:712:A:H2'	1:X:713:G:O4'	2.18	0.44
11:I:45:LYS:H	11:I:45:LYS:HD3	1.82	0.44
1:X:2339:A:H4'	11:I:56:LEU:HD21	2.00	0.44
1:X:1273:G:H2'	1:X:1274:C:O4'	2.18	0.44
1:X:1405:A:N6	19:Q:14:GLU:HG2	2.32	0.44
1:X:649:G:H22	1:X:660:G:N2	2.16	0.44
15:M:41:GLU:HG3	15:M:46:ARG:HD2	2.00	0.43
16:N:17:VAL:HG13	16:N:39:LEU:HD12	1.98	0.43
19:Q:62:ARG:O	19:Q:70:GLY:HA3	2.18	0.43
24:V:21:ARG:HG3	24:V:46:LEU:HD22	2.00	0.43
1:X:1421:U:H2'	1:X:1422:C:O4'	2.18	0.43
1:X:1547:U:H2'	1:X:1548:U:C6	2.53	0.43
1:X:1674:C:H2'	1:X:1675:C:C6	2.53	0.43
1:X:1979:C:H4'	1:X:1980:A:OP1	2.18	0.43
3:A:97:TYR:HE2	3:A:103:ARG:HB2	1.83	0.43
1:X:38:G:H21	5:C:42:THR:HG21	1.83	0.43
15:M:33:VAL:HG22	15:M:51:GLU:HB2	2.00	0.43
23:U:25:ARG:O	23:U:32:ARG:HD2	2.18	0.43
1:X:116:A:C8	1:X:117:A:C8	3.06	0.43
2:Y:39:C:H2'	14:L:97:HIS:HE1	1.83	0.43
1:X:875:G:O2'	2:Y:80:A:N3	2.44	0.43
5:C:6:VAL:HG12	5:C:7:ILE:HG12	1.99	0.43
6:D:35:VAL:HG22	6:D:90:THR:HG23	1.99	0.43
22:T:25:LYS:HB2	22:T:37:LEU:HB3	2.00	0.43
1:X:1307:U:H5"	1:X:1307:U:H6	1.83	0.43
1:X:2485:U:O2	1:X:2485:U:H2'	2.17	0.43
1:X:748:A:H5"	1:X:749:C:H5	1.84	0.43
1:X:748:A:H5'	1:X:749:C:OP2	2.19	0.43
18:P:39:ARG:HG3	18:P:97:VAL:HB	2.00	0.43
1:X:2310:G:H4'	22:T:43:THR:H	1.83	0.43
23:U:64:ALA:C	23:U:66:ALA:H	2.21	0.43
3:A:188:GLU:HG2	3:A:188:GLU:H	1.54	0.43
5:C:118:VAL:HG22	5:C:188:ILE:HD12	2.00	0.43
9:G:103:TYR:O	9:G:107:GLN:NE2	2.51	0.43
6:D:60:ILE:HB	6:D:99:PHE:HE1	1.83	0.43
1:X:1765:C:O5'	1:X:1765:C:H6	2.01	0.43
1:X:336:A:H2'	1:X:337:G:H8	1.83	0.43
11:I:28:LYS:NZ	11:I:36:GLY:CA	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:35:LYS:HA	19:Q:38:ILE:HG22	2.00	0.43
1:X:1574:A:O2'	1:X:1575:C:H3'	2.18	0.43
1:X:2186:G:H2'	1:X:2187:A:C8	2.54	0.43
1:X:2556:A:H5"	1:X:2557:G:H5'	2.00	0.43
1:X:577:U:O5'	1:X:956:A:N6	2.52	0.43
28:2:40:HIS:CA	28:2:41:GLN:CA	2.97	0.43
6:D:65:PRO:HA	6:D:89:VAL:HG13	2.01	0.43
4:B:77:ILE:HD13	15:M:3:THR:HG22	2.00	0.43
19:Q:28:TRP:CZ3	19:Q:77:LYS:HB2	2.53	0.43
1:X:1859:A:H2'	1:X:1860:A:C8	2.54	0.43
1:X:2270:U:H2'	1:X:2271:C:C6	2.53	0.43
1:X:517:A:C5'	1:X:518:A:H5'	2.48	0.43
2:Y:30:C:H2'	2:Y:31:A:H8	1.84	0.43
4:B:105:THR:HB	4:B:166:THR:HA	2.01	0.43
10:H:116:ARG:HG3	15:M:38:LYS:HE2	2.01	0.43
20:R:9:HIS:H	20:R:9:HIS:CD2	2.37	0.43
21:S:51:LEU:HD13	21:S:86:VAL:HG21	2.00	0.43
1:X:1329:U:H2'	1:X:1330:G:H8	1.84	0.43
1:X:890:U:H2'	1:X:891:A:H3'	2.00	0.43
3:A:108:PRO:HD2	3:A:111:LEU:HB2	2.01	0.43
10:H:113:PRO:HB3	10:H:132:GLU:HB3	2.01	0.43
11:I:102:LYS:O	11:I:104:ARG:N	2.52	0.43
23:U:51:ILE:HG12	23:U:59:THR:HB	2.00	0.43
1:X:460:U:O4	1:X:592:G:H1'	2.18	0.43
1:X:651:C:C2'	1:X:652:C:H5"	2.49	0.43
5:C:170:LEU:HA	5:C:171:PRO:HD3	1.84	0.42
2:Y:46:G:H4'	6:D:92:ARG:HH12	1.84	0.42
1:X:614:G:C8	11:I:98:LEU:HD21	2.53	0.42
1:X:590:C:H2'	1:X:591:G:H8	1.84	0.42
1:X:719:A:H2'	1:X:720:A:O4'	2.18	0.42
6:D:73:SER:O	6:D:79:LEU:HB3	2.19	0.42
9:G:102:ARG:O	9:G:102:ARG:HG2	2.19	0.42
23:U:78:ILE:HG12	23:U:79:GLU:H	1.85	0.42
1:X:1583:A:H3'	3:A:86:PRO:HG3	2.01	0.42
1:X:748:A:H3'	1:X:749:C:C6	2.53	0.42
11:I:83:LEU:HD23	11:I:84:GLU:H	1.84	0.42
12:J:26:ASP:HB3	12:J:27:TYR:H	1.61	0.42
12:J:78:LYS:HA	12:J:88:LYS:HZ3	1.84	0.42
17:O:36:LYS:NZ	17:O:54:TYR:HB3	2.35	0.42
1:X:1193:G:H2'	1:X:1194:U:C6	2.54	0.42
1:X:216:U:H2'	1:X:217:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:333:A:O4'	1:X:351:A:H1'	2.19	0.42
1:X:533:C:H1'	1:X:563:U:O2'	2.19	0.42
1:X:873:U:H1'	1:X:2247:A:H5"	2.00	0.42
3:A:231:HIS:HD2	3:A:233:HIS:N	2.11	0.42
1:X:1336:G:OP1	18:P:105:ARG:HD2	2.20	0.42
19:Q:66:GLY:O	19:Q:68:PHE:N	2.52	0.42
19:Q:68:PHE:C	19:Q:70:GLY:H	2.21	0.42
1:X:103:U:H2'	1:X:104:C:H6	1.82	0.42
1:X:1483:G:N2	1:X:1541:G:H1'	2.35	0.42
1:X:1779:C:OP1	3:A:222:ARG:NH1	2.52	0.42
1:X:1790:G:H5'	1:X:1811:A:N6	2.34	0.42
1:X:771:C:O2	1:X:1964:A:H2	2.03	0.42
1:X:1974:U:H2'	1:X:1975:G:H5"	2.00	0.42
1:X:394:U:H2'	1:X:395:G:C8	2.54	0.42
2:Y:78:A:H2'	2:Y:79:U:O4'	2.18	0.42
1:X:2015:G:O2'	4:B:145:LYS:HE2	2.20	0.42
9:G:107:GLN:C	9:G:109:GLY:N	2.72	0.42
10:H:77:THR:HA	10:H:94:ASN:HB3	2.00	0.42
22:T:23:VAL:HA	22:T:38:VAL:HG23	2.01	0.42
1:X:409:G:H1'	23:U:45:ASN:HD22	1.83	0.42
1:X:1339:U:H5"	1:X:1994:U:H1'	2.01	0.42
1:X:1493:A:H2'	1:X:1494:G:O4'	2.19	0.42
3:A:182:LEU:HB2	3:A:268:ARG:O	2.19	0.42
1:X:1384:G:N2	1:X:1385:C:H41	2.17	0.42
1:X:1687:C:H6	1:X:1687:C:O5'	2.01	0.42
1:X:2784:A:C6	1:X:2866:A:C8	3.07	0.42
9:G:107:GLN:C	9:G:109:GLY:H	2.23	0.42
9:G:98:LYS:HB3	9:G:116:ARG:HB2	2.01	0.42
15:M:33:VAL:HA	15:M:51:GLU:HB2	2.01	0.42
18:P:89:ARG:CZ	18:P:132:GLY:H	2.32	0.42
19:Q:53:ILE:HD13	19:Q:80:VAL:HG13	2.01	0.42
1:X:954:U:P	11:I:38:LYS:HG2	2.59	0.42
3:A:96:HIS:CE1	3:A:100:GLY:HA2	2.47	0.42
10:H:85:ASP:OD2	10:H:87:SER:HB3	2.20	0.42
16:N:88:ILE:CG1	17:O:49:GLU:HB2	2.48	0.42
21:S:23:ALA:HA	21:S:83:PHE:O	2.19	0.42
21:S:3:LEU:HB3	21:S:56:VAL:HA	2.02	0.42
1:X:1563:U:H2'	1:X:1564:U:C6	2.54	0.42
1:X:1736:C:H2'	1:X:1737:G:H8	1.84	0.42
1:X:2238:G:O4'	1:X:2406:C:H2'	2.20	0.42
1:X:520:C:H2'	1:X:520:C:O2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:542:A:H2	1:X:2004:U:O2'	2.01	0.42
1:X:852:U:H2'	1:X:853:C:C6	2.55	0.42
12:J:48:ILE:HD12	12:J:71:PRO:HG3	2.01	0.42
23:U:52:ARG:HD3	23:U:62:LEU:HD22	2.01	0.42
1:X:1441:A:H4'	1:X:1442:C:O5'	2.20	0.42
1:X:2237:C:O2'	1:X:2406:C:OP2	2.37	0.42
1:X:347:C:H2'	1:X:348:U:C6	2.54	0.42
1:X:56:C:H2'	1:X:57:G:O4'	2.19	0.42
1:X:616:U:H5'	1:X:617:U:OP2	2.20	0.42
1:X:693:A:H2'	1:X:694:G:C8	2.54	0.42
1:X:689:A:H2	1:X:815:A:H61	1.64	0.42
1:X:830:C:O2'	1:X:852:U:H5"	2.19	0.42
3:A:43:ARG:N	3:A:43:ARG:CD	2.83	0.42
4:B:177:ALA:C	4:B:179:GLU:H	2.24	0.42
9:G:33:ILE:O	9:G:69:ASP:OD1	2.38	0.42
12:J:82:THR:HB	12:J:83:ARG:H	1.76	0.42
12:J:88:LYS:HB3	12:J:89:GLY:H	1.59	0.42
19:Q:35:LYS:O	19:Q:38:ILE:HG22	2.20	0.42
1:X:101:A:H5"	1:X:102:C:H5	1.85	0.42
1:X:1128:G:H3'	1:X:1129:A:H5"	2.01	0.42
1:X:1033:G:N2	1:X:1153:A:H2	2.10	0.42
1:X:487:G:H4'	1:X:512:A:N1	2.34	0.42
4:B:85:ALA:H	4:B:86:PRO:HD2	1.85	0.41
9:G:106:TYR:O	9:G:108:GLY:N	2.48	0.41
1:X:2621:G:OP1	9:G:110:LEU:HD22	2.20	0.41
10:H:25:LEU:HD11	10:H:52:VAL:HG23	2.01	0.41
1:X:1219:C:H2'	1:X:1220:G:O4'	2.20	0.41
1:X:1644:G:H2'	1:X:1645:U:H6	1.85	0.41
1:X:2445:C:H5"	30:4:6:SER:HB3	2.01	0.41
1:X:339:U:O4	1:X:343:A:C8	2.73	0.41
1:X:649:G:N2	1:X:660:G:N2	2.68	0.41
3:A:88:ARG:O	3:A:89:SER:CB	2.68	0.41
4:B:5:LEU:HG	4:B:195:LEU:HD11	2.02	0.41
5:C:33:TRP:CD1	5:C:95:LEU:HB2	2.55	0.41
6:D:40:LEU:HB2	6:D:41:GLY:H	1.70	0.41
20:R:10:HIS:O	20:R:11:ASN:CB	2.68	0.41
1:X:534:U:H4'	1:X:564:U:H4'	2.01	0.41
1:X:679:C:H2'	1:X:680:U:C6	2.55	0.41
29:3:31:HIS:CA	29:3:32:GLN:CA	2.98	0.41
6:D:34:ILE:HG12	6:D:96:MET:HG3	2.02	0.41
1:X:2851:G:H4'	15:M:8:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:25:ASN:O	21:S:26:LYS:HB3	2.20	0.41
1:X:1276:U:H1'	26:Z:10:LYS:HG3	2.03	0.41
1:X:2226:A:H2'	1:X:2227:C:C6	2.55	0.41
3:A:67:PHE:CD2	3:A:153:ALA:HB3	2.56	0.41
15:M:55:ILE:O	15:M:103:LYS:O	2.38	0.41
17:O:56:VAL:HG12	17:O:97:GLY:HA3	2.02	0.41
1:X:85:C:H5"	20:R:42:ARG:HH21	1.85	0.41
25:W:45:LYS:O	25:W:48:LYS:HB2	2.19	0.41
1:X:1117:G:H2'	1:X:1118:G:H8	1.85	0.41
1:X:1437:A:H2'	1:X:1438:G:C8	2.55	0.41
1:X:1542:G:N2	1:X:1562:G:H1	1.99	0.41
1:X:2796:A:H2'	1:X:2797:G:C8	2.55	0.41
5:C:164:VAL:C	5:C:166:TRP:N	2.72	0.41
6:D:114:PHE:HZ	6:D:176:PRO:HG2	1.84	0.41
9:G:50:PRO:HG2	9:G:53:ARG:HG3	2.02	0.41
11:I:62:LYS:CE	11:I:64:GLY:HA2	2.45	0.41
12:J:42:TRP:CD1	12:J:97:VAL:HG12	2.56	0.41
14:L:26:ARG:HG2	14:L:86:GLN:HB3	2.02	0.41
16:N:93:LYS:CE	17:O:5:ILE:HD13	2.37	0.41
17:O:73:LYS:HB2	17:O:82:ARG:HB2	2.03	0.41
1:X:71:A:C5	24:V:54:ASN:HB3	2.55	0.41
1:X:1658:A:H2'	1:X:1659:G:O4'	2.21	0.41
1:X:1672:A:H3'	1:X:1673:C:C6	2.55	0.41
1:X:2266:A:C2	1:X:2325:A:N6	2.81	0.41
1:X:2736:U:H1'	1:X:2737:A:H5"	2.02	0.41
1:X:922:A:N1	1:X:2256:G:H1'	2.34	0.41
4:B:149:ARG:CZ	9:G:106:TYR:CD1	3.02	0.41
4:B:4:ILE:HD13	4:B:28:ALA:HB1	2.02	0.41
1:X:203:G:H1'	1:X:205:A:N6	2.32	0.41
1:X:2292:C:H5"	6:D:88:LYS:HD3	2.01	0.41
1:X:572:G:H22	1:X:587:A:H2	1.68	0.41
3:A:169:GLU:HB3	3:A:170:SER:H	1.63	0.41
1:X:2035:G:N2	4:B:148:GLY:O	2.48	0.41
12:J:36:ILE:HD12	12:J:133:VAL:HG21	2.02	0.41
17:O:5:ILE:CD1	17:O:6:GLN:H	2.19	0.41
1:X:829:C:H2'	1:X:830:C:H6	1.86	0.41
3:A:134:ARG:HG3	3:A:135:PHE:HD2	1.86	0.41
6:D:92:ARG:HB2	6:D:92:ARG:NH2	2.36	0.41
12:J:14:PHE:HE1	12:J:90:ALA:CA	2.28	0.41
20:R:110:SER:OG	20:R:111:GLY:N	2.52	0.41
20:R:84:VAL:HG23	20:R:88:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:59:LEU:HD12	22:T:79:ILE:HD12	2.02	0.41
25:W:12:ARG:HG3	25:W:50:LEU:HD21	2.03	0.41
1:X:2508:G:H5"	1:X:2509:A:H5"	2.01	0.41
18:P:25:PHE:C	18:P:25:PHE:CD2	2.94	0.41
21:S:13:LYS:HB2	21:S:18:MET:HB2	2.03	0.41
22:T:14:ARG:HG3	22:T:15:ASP:N	2.36	0.41
22:T:48:GLY:H	22:T:51:VAL:HB	1.86	0.41
4:B:149:ARG:NH1	9:G:106:TYR:HB2	2.36	0.41
4:B:5:LEU:HD22	4:B:49:ILE:HG22	2.02	0.41
7:E:48:ASP:HB3	7:E:49:GLN:HE21	1.86	0.41
11:I:28:LYS:HZ2	11:I:36:GLY:HA2	1.86	0.41
19:Q:12:ILE:O	19:Q:16:ALA:HB3	2.20	0.41
20:R:7:GLY:HA3	20:R:42:ARG:O	2.20	0.41
23:U:22:GLY:H	23:U:39:LYS:HB2	1.85	0.41
1:X:1378:A:H2'	1:X:1378:A:N3	2.36	0.41
1:X:2206:C:H1'	3:A:262:LYS:HE3	2.02	0.41
1:X:2552:C:H5"	1:X:2553:G:H5"	2.03	0.41
4:B:67:PHE:CE1	4:B:75:THR:HG22	2.56	0.41
5:C:3:GLN:CG	5:C:116:LYS:HD2	2.51	0.41
5:C:146:GLU:HB3	5:C:184:ASP:HB2	2.03	0.41
10:H:27:SER:HA	10:H:50:ILE:HD12	2.02	0.41
1:X:986:A:O3'	16:N:48:ARG:NH1	2.54	0.41
1:X:1443:G:H2'	1:X:1444:C:H6	1.86	0.41
1:X:1582:A:OP1	3:A:211:ARG:NH2	2.48	0.41
1:X:1997:A:H2'	1:X:1998:A:C8	2.56	0.41
1:X:2407:G:H5"	1:X:2408:G:OP1	2.21	0.41
1:X:2869:U:H2'	1:X:2870:C:C6	2.56	0.41
4:B:14:ILE:HG22	4:B:21:ILE:HB	2.04	0.40
1:X:654:A:H2'	1:X:654:A:N3	2.36	0.40
26:Z:51:TYR:HA	26:Z:55:ARG:HA	2.03	0.40
5:C:166:TRP:HB3	5:C:167:VAL:H	1.63	0.40
22:T:14:ARG:CG	22:T:15:ASP:H	2.34	0.40
23:U:14:VAL:O	23:U:15:VAL:HG22	2.21	0.40
1:X:1623:C:H4'	1:X:1624:A:O5'	2.21	0.40
1:X:2561:G:H8	1:X:2561:G:H5'	1.86	0.40
1:X:88:G:H3'	1:X:89:A:H5"	2.04	0.40
9:G:162:LYS:N	9:G:163:PRO:CD	2.85	0.40
12:J:79:PRO:CD	12:J:88:LYS:HD2	2.50	0.40
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.54	0.40
19:Q:68:PHE:C	19:Q:70:GLY:N	2.75	0.40
19:Q:89:GLU:HB3	19:Q:90:ALA:H	1.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:108:VAL:HB	20:R:109:ALA:H	1.49	0.40
21:S:95:SER:HB3	21:S:119:ASN:HD22	1.86	0.40
23:U:21:ARG:HG2	23:U:40:ARG:HG2	2.04	0.40
1:X:10:A:H2'	1:X:11:G:C8	2.56	0.40
1:X:70:A:H5'	1:X:71:A:C3'	2.44	0.40
2:Y:58:G:H4'	2:Y:59:A:H5"	2.04	0.40
2:Y:64:C:H2'	2:Y:65:A:C8	2.56	0.40
5:C:188:ILE:H	5:C:188:ILE:HG13	1.42	0.40
1:X:923:A:C5	12:J:12:LYS:HE3	2.57	0.40
1:X:463:C:N4	1:X:467:U:H5	2.08	0.40
1:X:1016:C:O2'	9:G:56:THR:HG21	2.21	0.40
11:I:72:TYR:CE2	11:I:105:PRO:HB2	2.57	0.40
12:J:54:VAL:CG1	12:J:121:LEU:HB3	2.52	0.40
14:L:15:ARG:HA	14:L:15:ARG:HD3	1.93	0.40
14:L:67:THR:O	14:L:70:ALA:HB3	2.22	0.40
25:W:3:ILE:O	25:W:31:SER:HA	2.22	0.40
1:X:1004:A:H5'	17:O:71:ILE:HD11	2.04	0.40
1:X:1467:U:H3'	1:X:1467:U:C6	2.54	0.40
1:X:682:G:C2'	1:X:682:G:N3	2.83	0.40
1:X:811:G:OP2	5:C:56:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	238/274 (87%)	170 (71%)	39 (16%)	29 (12%)	0 2
4	B	203/211 (96%)	172 (85%)	17 (8%)	14 (7%)	1 8
5	C	195/205 (95%)	131 (67%)	37 (19%)	27 (14%)	0 1
6	D	175/180 (97%)	136 (78%)	26 (15%)	13 (7%)	1 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	E	169/185 (91%)	132 (78%)	29 (17%)	8 (5%)	2 17
8	F	69/144 (48%)	59 (86%)	8 (12%)	2 (3%)	4 28
9	G	140/174 (80%)	103 (74%)	23 (16%)	14 (10%)	0 3
10	H	132/134 (98%)	117 (89%)	9 (7%)	6 (4%)	2 18
11	I	139/156 (89%)	79 (57%)	34 (24%)	26 (19%)	0 0
12	J	134/141 (95%)	97 (72%)	26 (19%)	11 (8%)	1 5
13	K	111/116 (96%)	96 (86%)	7 (6%)	8 (7%)	1 7
14	L	102/114 (90%)	72 (71%)	20 (20%)	10 (10%)	0 3
15	M	106/166 (64%)	95 (90%)	7 (7%)	4 (4%)	3 22
16	N	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3 24
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0 1
18	P	125/134 (93%)	114 (91%)	5 (4%)	6 (5%)	2 17
19	Q	91/95 (96%)	59 (65%)	19 (21%)	13 (14%)	0 1
20	R	108/115 (94%)	66 (61%)	23 (21%)	19 (18%)	0 0
21	S	173/237 (73%)	145 (84%)	20 (12%)	8 (5%)	2 18
22	T	82/91 (90%)	64 (78%)	9 (11%)	9 (11%)	0 2
23	U	70/81 (86%)	39 (56%)	17 (24%)	14 (20%)	0 0
24	V	64/67 (96%)	57 (89%)	3 (5%)	4 (6%)	1 10
25	W	53/55 (96%)	49 (92%)	4 (8%)	0	100 100
26	Z	56/60 (93%)	47 (84%)	5 (9%)	4 (7%)	1 8
30	4	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1 14
All	All	2977/3390 (88%)	2294 (77%)	415 (14%)	268 (9%)	1 4

All (268) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	60	ARG
3	A	151	LYS
3	A	170	SER
3	A	187	SER
3	A	199	ALA
3	A	248	THR
3	A	250	TRP
3	A	271	VAL
4	B	76	ARG

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Mol	Chain	Res	Type
4	B	86	PRO
4	B	122	PHE
5	C	20	PRO
5	C	64	THR
5	C	67	ALA
5	C	129	LYS
5	C	163	ASN
5	C	164	VAL
5	C	172	VAL
7	E	126	PRO
9	G	33	ILE
9	G	37	ASP
9	G	67	ARG
9	G	91	THR
9	G	97	ASP
9	G	104	THR
9	G	107	GLN
9	G	158	HIS
9	G	170	PRO
10	H	27	SER
10	H	29	ILE
11	I	17	LYS
11	I	18	ARG
11	I	37	GLN
11	I	39	SER
11	I	48	PHE
11	I	56	LEU
11	I	59	ARG
11	I	62	LYS
11	I	86	THR
11	I	98	LEU
11	I	103	ASN
12	J	13	GLN
12	J	26	ASP
12	J	83	ARG
12	J	89	GLY
12	J	136	GLU
13	K	6	ALA
13	K	8	ARG
13	K	95	THR
14	L	21	THR
14	L	40	ALA

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Mol	Chain	Res	Type
14	L	68	ALA
14	L	95	LYS
15	M	27	PHE
15	M	29	PRO
16	N	7	GLY
16	N	8	ILE
16	N	92	ARG
17	O	10	LYS
17	O	31	ASP
17	O	97	GLY
18	P	9	ARG
18	P	50	VAL
19	Q	12	ILE
19	Q	13	SER
19	Q	67	ARG
19	Q	69	ILE
19	Q	84	GLU
20	R	11	ASN
20	R	62	MET
20	R	66	GLN
20	R	82	ALA
20	R	98	ILE
20	R	108	VAL
21	S	26	LYS
21	S	156	GLU
22	T	15	ASP
22	T	19	LYS
23	U	15	VAL
23	U	27	ASP
23	U	47	HIS
23	U	48	LYS
23	U	60	VAL
24	V	2	LYS
26	Z	4	HIS
3	A	54	ILE
3	A	98	ALA
3	A	197	GLY
3	A	198	ASN
3	A	220	HIS
4	B	121	ASN
4	B	123	ALA
4	B	132	LYS

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Mol	Chain	Res	Type
4	B	135	HIS
4	B	146	THR
5	C	9	GLN
5	C	22	VAL
5	C	55	GLY
5	C	60	GLY
5	C	121	ASP
5	C	125	ILE
5	C	127	ASP
5	C	165	SER
5	C	195	ILE
6	D	4	LEU
6	D	9	ASN
6	D	121	ALA
6	D	124	GLY
7	E	19	ALA
10	H	31	GLY
11	I	19	VAL
11	I	47	ALA
11	I	49	PHE
12	J	17	ARG
12	J	21	ASP
12	J	60	ARG
12	J	80	ALA
13	K	14	SER
13	K	92	GLY
14	L	45	ASP
14	L	92	GLY
15	M	41	GLU
16	N	87	ASN
17	O	30	GLY
17	O	48	GLY
19	Q	6	ILE
19	Q	63	LYS
20	R	5	SER
20	R	6	ALA
20	R	7	GLY
20	R	60	PRO
21	S	57	GLU
21	S	88	TYR
21	S	91	PRO
22	T	5	LYS

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Mol	Chain	Res	Type
22	T	14	ARG
23	U	19	ILE
23	U	30	VAL
23	U	41	VAL
23	U	55	GLY
23	U	78	ILE
26	Z	36	CYS
26	Z	37	HIS
30	4	20	HIS
3	A	109	GLU
3	A	206	LEU
3	A	219	PRO
3	A	249	PRO
3	A	263	ARG
4	B	73	ALA
4	B	74	PRO
5	C	15	ILE
5	C	173	ALA
5	C	189	ASP
5	C	190	ALA
6	D	5	LYS
6	D	122	PHE
7	E	55	PRO
7	E	119	ALA
7	E	173	ALA
9	G	34	PRO
9	G	68	PRO
10	H	41	ASN
11	I	54	SER
11	I	65	PHE
11	I	82	ASP
13	K	93	GLY
14	L	52	ALA
14	L	96	TYR
17	O	43	GLU
18	P	20	LEU
18	P	80	LEU
18	P	131	LYS
19	Q	61	LYS
19	Q	86	GLN
19	Q	87	SER
20	R	49	GLU

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Mol	Chain	Res	Type
20	R	85	ASP
20	R	87	GLU
20	R	110	SER
24	V	3	PRO
24	V	10	GLN
26	Z	53	ASP
3	A	35	GLU
3	A	45	ASN
3	A	89	SER
3	A	127	LEU
3	A	254	THR
3	A	269	PHE
4	B	85	ALA
4	B	137	ARG
5	C	13	ARG
6	D	10	ASP
6	D	40	LEU
6	D	52	LYS
7	E	7	GLN
7	E	13	SER
10	H	5	GLN
11	I	28	LYS
11	I	88	PHE
11	I	115	SER
13	K	4	GLY
14	L	53	ALA
17	O	9	GLY
17	O	28	GLU
17	O	29	ALA
17	O	49	GLU
19	Q	3	HIS
19	Q	4	TYR
20	R	16	PHE
20	R	63	THR
21	S	58	GLY
21	S	125	PRO
22	T	74	LYS
23	U	34	THR
23	U	42	GLN
23	U	76	LYS
3	A	55	GLY
3	A	244	ARG

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Mol	Chain	Res	Type
3	A	270	ILE
5	C	196	VAL
6	D	21	GLY
6	D	42	SER
6	D	71	LYS
6	D	81	GLN
7	E	59	GLN
9	G	165	VAL
10	H	42	LYS
11	I	8	PRO
11	I	9	THR
11	I	131	LYS
12	J	11	ARG
12	J	84	MET
13	K	10	LEU
14	L	33	ARG
17	O	7	THR
17	O	36	LYS
19	Q	5	ASP
20	R	31	GLY
20	R	111	GLY
22	T	7	VAL
23	U	12	ASN
4	B	17	ASN
4	B	75	THR
5	C	11	GLY
5	C	126	ALA
8	F	143	ASN
11	I	29	THR
17	O	11	GLN
21	S	6	LYS
30	4	5	SER
9	G	163	PRO
11	I	68	VAL
24	V	64	GLY
3	A	47	GLY
3	A	252	LYS
5	C	41	GLY
5	C	103	GLY
8	F	118	GLY
18	P	132	GLY
20	R	64	ASN

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Mol	Chain	Res	Type
22	T	13	GLY
22	T	73	GLY
5	C	171	PRO
9	G	157	PRO
11	I	57	ILE
15	M	74	GLY
22	T	27	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	185/215 (86%)	144 (78%)	41 (22%)	1 4
4	B	155/157 (99%)	135 (87%)	20 (13%)	4 19
5	C	157/163 (96%)	125 (80%)	32 (20%)	1 6
6	D	153/156 (98%)	129 (84%)	24 (16%)	2 12
7	E	136/144 (94%)	117 (86%)	19 (14%)	3 16
8	F	51/107 (48%)	46 (90%)	5 (10%)	8 31
9	G	118/146 (81%)	95 (80%)	23 (20%)	1 7
10	H	103/103 (100%)	81 (79%)	22 (21%)	1 5
11	I	108/121 (89%)	72 (67%)	36 (33%)	0 0
12	J	110/115 (96%)	93 (84%)	17 (16%)	2 12
13	K	90/93 (97%)	73 (81%)	17 (19%)	1 8
14	L	74/82 (90%)	54 (73%)	20 (27%)	0 1
15	M	94/134 (70%)	75 (80%)	19 (20%)	1 6
16	N	96/97 (99%)	81 (84%)	15 (16%)	2 12
17	O	75/79 (95%)	60 (80%)	15 (20%)	1 6
18	P	109/115 (95%)	94 (86%)	15 (14%)	3 16
19	Q	75/76 (99%)	60 (80%)	15 (20%)	1 6
20	R	91/96 (95%)	71 (78%)	20 (22%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	S	149/192 (78%)	126 (85%)	23 (15%)	2 13
22	T	62/67 (92%)	53 (86%)	9 (14%)	3 15
23	U	57/66 (86%)	33 (58%)	24 (42%)	0 0
24	V	54/55 (98%)	44 (82%)	10 (18%)	1 8
25	W	48/48 (100%)	38 (79%)	10 (21%)	1 6
26	Z	51/53 (96%)	37 (72%)	14 (28%)	0 1
30	4	35/35 (100%)	31 (89%)	4 (11%)	5 24
All	All	2436/2715 (90%)	1967 (81%)	469 (19%)	1 8

All (469) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	33	LEU
3	A	34	THR
3	A	35	GLU
3	A	39	LYS
3	A	40	THR
3	A	43	ARG
3	A	44	ASN
3	A	46	ARG
3	A	48	ARG
3	A	49	ILE
3	A	50	THR
3	A	52	ARG
3	A	54	ILE
3	A	61	LEU
3	A	68	LYS
3	A	69	ARG
3	A	92	ILE
3	A	105	ILE
3	A	108	PRO
3	A	111	LEU
3	A	131	LEU
3	A	133	LEU
3	A	151	LYS
3	A	157	ARG
3	A	164	GLN
3	A	175	VAL
3	A	183	ARG
3	A	203	ASN

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Mol	Chain	Res	Type
3	A	208	LYS
3	A	214	TRP
3	A	215	LEU
3	A	217	ARG
3	A	218	LYS
3	A	226	MET
3	A	240	THR
3	A	244	ARG
3	A	248	THR
3	A	252	LYS
3	A	259	THR
3	A	260	ARG
3	A	270	ILE
4	B	5	LEU
4	B	14	ILE
4	B	37	LYS
4	B	49	ILE
4	B	69	LYS
4	B	82	ARG
4	B	87	ASP
4	B	105	THR
4	B	111	LYS
4	B	119	ARG
4	B	131	SER
4	B	133	LYS
4	B	134	TRP
4	B	137	ARG
4	B	149	ARG
4	B	150	VAL
4	B	168	GLN
4	B	179	GLU
4	B	184	VAL
4	B	203	LYS
5	C	5	ASN
5	C	10	ASN
5	C	13	ARG
5	C	14	THR
5	C	15	ILE
5	C	31	VAL
5	C	40	ARG
5	C	45	THR
5	C	48	ARG

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Mol	Chain	Res	Type
5	C	51	VAL
5	C	53	LYS
5	C	74	VAL
5	C	90	SER
5	C	95	LEU
5	C	101	GLN
5	C	102	LEU
5	C	104	LEU
5	C	117	LEU
5	C	124	ASP
5	C	134	ILE
5	C	138	LYS
5	C	143	ASP
5	C	148	VAL
5	C	150	LEU
5	C	153	ASP
5	C	154	ASP
5	C	155	GLU
5	C	164	VAL
5	C	166	TRP
5	C	175	VAL
5	C	180	ILE
5	C	188	ILE
6	D	40	LEU
6	D	45	GLU
6	D	57	LEU
6	D	67	ILE
6	D	74	ILE
6	D	80	ARG
6	D	89	VAL
6	D	92	ARG
6	D	106	ILE
6	D	112	ARG
6	D	115	ARG
6	D	117	ILE
6	D	125	ARG
6	D	129	ASN
6	D	130	LEU
6	D	135	GLN
6	D	136	LEU
6	D	140	GLU
6	D	142	THR

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Mol	Chain	Res	Type
6	D	145	MET
6	D	147	ASP
6	D	150	ARG
6	D	163	ASP
6	D	175	LEU
7	E	11	VAL
7	E	33	LEU
7	E	35	VAL
7	E	38	ASN
7	E	44	ARG
7	E	49	GLN
7	E	50	LEU
7	E	57	ASP
7	E	64	LEU
7	E	67	LEU
7	E	68	THR
7	E	69	ARG
7	E	90	ARG
7	E	92	VAL
7	E	113	VAL
7	E	116	GLU
7	E	132	ASP
7	E	140	LEU
7	E	152	ARG
8	F	76	TYR
8	F	100	ASN
8	F	101	TRP
8	F	111	LYS
8	F	115	LEU
9	G	31	THR
9	G	37	ASP
9	G	38	GLU
9	G	41	TRP
9	G	53	ARG
9	G	62	ILE
9	G	71	THR
9	G	75	ILE
9	G	93	LYS
9	G	95	LEU
9	G	102	ARG
9	G	104	THR
9	G	113	GLU

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Mol	Chain	Res	Type
9	G	116	ARG
9	G	126	VAL
9	G	132	PHE
9	G	145	HIS
9	G	146	THR
9	G	154	GLU
9	G	165	VAL
9	G	166	LEU
9	G	168	THR
9	G	169	GLN
10	H	3	MET
10	H	8	LEU
10	H	18	GLU
10	H	20	MET
10	H	25	LEU
10	H	26	ASN
10	H	27	SER
10	H	32	LYS
10	H	36	THR
10	H	41	ASN
10	H	47	VAL
10	H	81	ILE
10	H	83	ARG
10	H	87	SER
10	H	89	ILE
10	H	94	ASN
10	H	106	ARG
10	H	116	ARG
10	H	117	GLU
10	H	120	ASP
10	H	122	ARG
10	H	129	LEU
11	I	7	LYS
11	I	12	SER
11	I	13	ARG
11	I	19	VAL
11	I	27	ASP
11	I	29	THR
11	I	32	ARG
11	I	34	HIS
11	I	35	LYS
11	I	37	GLN

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Mol	Chain	Res	Type
11	I	38	LYS
11	I	39	SER
11	I	40	ARG
11	I	45	LYS
11	I	53	ARG
11	I	56	LEU
11	I	57	ILE
11	I	59	ARG
11	I	60	LEU
11	I	65	PHE
11	I	78	SER
11	I	83	LEU
11	I	84	GLU
11	I	85	ASP
11	I	88	PHE
11	I	96	TYR
11	I	98	LEU
11	I	101	ARG
11	I	103	ASN
11	I	106	VAL
11	I	107	LYS
11	I	113	GLU
11	I	114	ILE
11	I	120	VAL
11	I	123	ASP
11	I	142	LEU
12	J	8	THR
12	J	10	PHE
12	J	11	ARG
12	J	19	THR
12	J	21	ASP
12	J	26	ASP
12	J	27	TYR
12	J	49	GLU
12	J	61	ARG
12	J	64	LYS
12	J	81	GLU
12	J	91	VAL
12	J	94	TRP
12	J	113	GLU
12	J	132	MET
12	J	133	VAL

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Mol	Chain	Res	Type
12	J	134	LYS
13	K	5	LYS
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	35	GLN
13	K	45	ARG
13	K	51	LEU
13	K	53	THR
13	K	83	VAL
13	K	94	TYR
13	K	95	THR
13	K	99	ARG
13	K	102	THR
13	K	109	THR
14	L	8	ARG
14	L	11	LEU
14	L	12	ARG
14	L	13	THR
14	L	18	ARG
14	L	31	VAL
14	L	33	ARG
14	L	36	LYS
14	L	37	HIS
14	L	38	ILE
14	L	43	ILE
14	L	45	ASP
14	L	47	ARG
14	L	64	LYS
14	L	66	ASP
14	L	71	VAL
14	L	89	PHE
14	L	91	ARG
14	L	93	SER
14	L	108	ARG
15	M	2	GLN
15	M	5	ILE
15	M	6	LYS
15	M	11	GLU

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Mol	Chain	Res	Type
15	M	12	LEU
15	M	13	LEU
15	M	19	ASP
15	M	22	ARG
15	M	31	ASP
15	M	34	ARG
15	M	37	THR
15	M	51	GLU
15	M	63	ARG
15	M	79	ARG
15	M	91	VAL
15	M	92	THR
15	M	96	ARG
15	M	99	VAL
15	M	101	ARG
16	N	8	ILE
16	N	16	LYS
16	N	18	LEU
16	N	19	LYS
16	N	22	LYS
16	N	30	LYS
16	N	51	ARG
16	N	71	LEU
16	N	78	THR
16	N	88	ILE
16	N	90	LEU
16	N	91	ASN
16	N	93	LYS
16	N	97	ASP
16	N	104	GLU
17	O	7	THR
17	O	14	VAL
17	O	18	ASP
17	O	22	VAL
17	O	26	GLN
17	O	28	GLU
17	O	39	PHE
17	O	40	VAL
17	O	55	THR
17	O	56	VAL
17	O	65	ARG
17	O	69	ILE

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Mol	Chain	Res	Type
17	O	81	ARG
17	O	88	GLN
17	O	96	LEU
18	P	16	GLN
18	P	17	GLN
18	P	25	PHE
18	P	32	ARG
18	P	37	LYS
18	P	45	ILE
18	P	50	VAL
18	P	89	ARG
18	P	116	ILE
18	P	118	LYS
18	P	120	ARG
18	P	124	ILE
18	P	125	THR
18	P	126	ILE
18	P	133	ASN
19	Q	7	LEU
19	Q	8	GLN
19	Q	12	ILE
19	Q	14	GLU
19	Q	26	SER
19	Q	37	GLU
19	Q	38	ILE
19	Q	42	ILE
19	Q	61	LYS
19	Q	63	LYS
19	Q	65	VAL
19	Q	69	ILE
19	Q	71	GLN
19	Q	79	ILE
19	Q	84	GLU
20	R	11	ASN
20	R	18	LYS
20	R	23	ILE
20	R	25	LEU
20	R	26	SER
20	R	32	GLN
20	R	37	LEU
20	R	38	LEU
20	R	42	ARG

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Mol	Chain	Res	Type
20	R	44	GLN
20	R	71	GLN
20	R	73	GLU
20	R	79	SER
20	R	80	LYS
20	R	95	ARG
20	R	98	ILE
20	R	104	VAL
20	R	105	ARG
20	R	106	VAL
20	R	108	VAL
21	S	3	LEU
21	S	13	LYS
21	S	18	MET
21	S	22	VAL
21	S	26	LYS
21	S	29	ASN
21	S	51	LEU
21	S	65	LEU
21	S	67	LYS
21	S	71	MET
21	S	82	ASP
21	S	88	TYR
21	S	100	THR
21	S	120	LEU
21	S	123	VAL
21	S	128	ARG
21	S	132	GLN
21	S	134	LEU
21	S	159	THR
21	S	160	LEU
21	S	166	LEU
21	S	169	VAL
21	S	175	ARG
22	T	5	LYS
22	T	16	SER
22	T	17	ASN
22	T	37	LEU
22	T	38	VAL
22	T	62	LEU
22	T	63	SER
22	T	64	ASP

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Mol	Chain	Res	Type
22	T	85	GLN
23	U	8	THR
23	U	10	LYS
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	21	ARG
23	U	23	LYS
23	U	32	ARG
23	U	35	THR
23	U	37	ILE
23	U	42	GLN
23	U	43	ARG
23	U	46	LEU
23	U	49	LYS
23	U	54	ASN
23	U	56	GLN
23	U	63	SER
23	U	65	ASN
23	U	67	LEU
23	U	69	THR
23	U	76	LYS
24	V	1	MET
24	V	7	ARG
24	V	13	ASP
24	V	14	PHE
24	V	19	ASP
24	V	21	ARG
24	V	25	LEU
24	V	41	HIS
24	V	49	GLU
24	V	65	GLU
25	W	2	LYS
25	W	4	LYS
25	W	9	VAL
25	W	10	ILE
25	W	12	ARG
25	W	15	ASN
25	W	30	ASP

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Mol	Chain	Res	Type
25	W	32	ARG
25	W	34	VAL
25	W	36	ASP
26	Z	3	LYS
26	Z	4	HIS
26	Z	6	VAL
26	Z	8	LYS
26	Z	18	MET
26	Z	19	ARG
26	Z	31	THR
26	Z	35	GLN
26	Z	40	LYS
26	Z	41	LEU
26	Z	53	ASP
26	Z	55	ARG
26	Z	57	VAL
26	Z	58	LEU
30	4	2	LYS
30	4	9	LYS
30	4	14	CYS
30	4	30	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	96	HIS
3	A	201	HIS
3	A	231	HIS
4	B	129	HIS
4	B	180	ASN
5	C	5	ASN
5	C	61	GLN
5	C	66	ASN
5	C	176	ASN
6	D	9	ASN
7	E	38	ASN
7	E	49	GLN
7	E	106	ASN
7	E	143	GLN
9	G	76	GLN
10	H	26	ASN
10	H	41	ASN

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Mol	Chain	Res	Type
11	I	37	GLN
14	L	41	GLN
14	L	49	GLN
14	L	97	HIS
15	M	20	HIS
15	M	48	GLN
16	N	31	GLN
16	N	66	ASN
16	N	75	ASN
16	N	81	ASN
16	N	91	ASN
17	O	11	GLN
17	O	79	GLN
17	O	88	GLN
18	P	13	GLN
18	P	16	GLN
18	P	17	GLN
18	P	78	ASN
18	P	81	HIS
18	P	115	ASN
19	Q	71	GLN
20	R	15	HIS
20	R	69	GLN
21	S	80	HIS
21	S	119	ASN
21	S	132	GLN
22	T	17	ASN
22	T	35	ASN
23	U	42	GLN
23	U	47	HIS
24	V	41	HIS
25	W	49	HIS
26	Z	43	HIS
26	Z	44	HIS
30	4	36	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2681/2880 (93%)	638 (23%)	238 (8%)
2	Y	121/123 (98%)	28 (23%)	5 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2802/3003 (93%)	666 (23%)	243 (8%)

All (666) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	3	U
1	X	4	C
1	X	13	A
1	X	14	A
1	X	33	C
1	X	34	U
1	X	45	C
1	X	48	A
1	X	49	U
1	X	50	G
1	X	51	A
1	X	54	G
1	X	63	A
1	X	69	G
1	X	70	A
1	X	71	A
1	X	72	A
1	X	74	G
1	X	82	G
1	X	83	A
1	X	87	G
1	X	89	A
1	X	90	G
1	X	91	A
1	X	95	G
1	X	97	U
1	X	98	U
1	X	99	U
1	X	100	G
1	X	101	A
1	X	105	G
1	X	107	G
1	X	116	A
1	X	117	A
1	X	118	U
1	X	123	A

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Mol	Chain	Res	Type
1	X	124	A
1	X	125	A
1	X	127	C
1	X	129	A
1	X	136	A
1	X	138	G
1	X	143	A
1	X	147	G
1	X	149	A
1	X	154	U
1	X	155	G
1	X	157	G
1	X	158	A
1	X	173	A
1	X	176	A
1	X	177	U
1	X	192	G
1	X	193	A
1	X	194	G
1	X	199	A
1	X	204	A
1	X	206	U
1	X	207	U
1	X	210	A
1	X	222	G
1	X	225	G
1	X	229	G
1	X	242	A
1	X	243	G
1	X	245	C
1	X	246	C
1	X	248	A
1	X	304	A
1	X	305	A
1	X	306	G
1	X	310	A
1	X	312	G
1	X	313	U
1	X	321	A
1	X	322	A
1	X	323	G
1	X	328	A

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Mol	Chain	Res	Type
1	X	333	A
1	X	335	A
1	X	340	G
1	X	341	A
1	X	342	G
1	X	343	A
1	X	344	G
1	X	358	C
1	X	388	G
1	X	393	U
1	X	397	U
1	X	399	G
1	X	400	U
1	X	409	G
1	X	414	A
1	X	418	C
1	X	419	G
1	X	424	G
1	X	425	A
1	X	441	A
1	X	456	C
1	X	459	A
1	X	461	A
1	X	463	C
1	X	466	A
1	X	467	U
1	X	468	A
1	X	469	G
1	X	486	U
1	X	491	A
1	X	492	G
1	X	504	G
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	523	A
1	X	539	A
1	X	540	G
1	X	541	C

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Mol	Chain	Res	Type
1	X	542	A
1	X	543	G
1	X	554	U
1	X	555	U
1	X	556	A
1	X	558	G
1	X	559	C
1	X	560	G
1	X	572	G
1	X	577	U
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	600	G
1	X	613	A
1	X	614	G
1	X	617	U
1	X	623	G
1	X	624	A
1	X	625	A
1	X	626	A
1	X	627	A
1	X	628	A
1	X	633	G
1	X	638	A
1	X	645	G
1	X	648	A
1	X	649	G
1	X	651	C
1	X	652	C
1	X	654	A
1	X	655	A
1	X	656	U
1	X	657	A
1	X	664	C
1	X	665	A
1	X	667	U
1	X	669	G
1	X	682	G

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Mol	Chain	Res	Type
1	X	683	A
1	X	684	C
1	X	698	A
1	X	699	G
1	X	700	C
1	X	728	G
1	X	729	A
1	X	730	C
1	X	731	A
1	X	732	G
1	X	736	G
1	X	743	A
1	X	747	A
1	X	751	G
1	X	752	G
1	X	753	U
1	X	758	G
1	X	759	C
1	X	760	U
1	X	777	A
1	X	778	G
1	X	780	U
1	X	781	G
1	X	788	G
1	X	789	G
1	X	790	A
1	X	795	A
1	X	797	A
1	X	798	G
1	X	802	A
1	X	803	C
1	X	804	C
1	X	805	G
1	X	806	A
1	X	814	G
1	X	815	A
1	X	818	G
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	858	G

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Mol	Chain	Res	Type
1	X	859	U
1	X	872	G
1	X	879	A
1	X	880	C
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	944	A
1	X	952	A
1	X	955	G
1	X	956	A
1	X	957	G
1	X	969	U
1	X	970	A
1	X	972	C
1	X	973	U
1	X	985	G
1	X	994	A
1	X	995	A
1	X	1000	G
1	X	1001	A
1	X	1006	C
1	X	1007	A
1	X	1014	G
1	X	1016	C
1	X	1022	A
1	X	1023	U
1	X	1024	G
1	X	1028	G
1	X	1031	C
1	X	1032	A
1	X	1033	G
1	X	1034	U
1	X	1036	G
1	X	1037	U
1	X	1038	U
1	X	1044	U
1	X	1051	U
1	X	1053	G

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Mol	Chain	Res	Type
1	X	1054	C
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1058	G
1	X	1060	C
1	X	1068	A
1	X	1073	G
1	X	1077	U
1	X	1078	A
1	X	1081	A
1	X	1082	G
1	X	1086	C
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	1108	U
1	X	1115	C
1	X	1121	G
1	X	1122	A
1	X	1123	G
1	X	1128	G
1	X	1129	A
1	X	1130	U
1	X	1139	A
1	X	1140	A
1	X	1141	U
1	X	1142	G
1	X	1143	A
1	X	1145	C
1	X	1146	G
1	X	1152	C
1	X	1153	A
1	X	1154	A
1	X	1155	G
1	X	1161	U
1	X	1183	C
1	X	1185	C

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Mol	Chain	Res	Type
1	X	1187	A
1	X	1188	A
1	X	1189	G
1	X	1191	G
1	X	1192	A
1	X	1194	U
1	X	1195	U
1	X	1223	G
1	X	1224	A
1	X	1233	A
1	X	1234	C
1	X	1240	G
1	X	1250	A
1	X	1251	G
1	X	1265	G
1	X	1266	G
1	X	1269	G
1	X	1275	A
1	X	1281	A
1	X	1284	G
1	X	1285	A
1	X	1286	U
1	X	1288	A
1	X	1289	A
1	X	1297	A
1	X	1299	A
1	X	1300	A
1	X	1302	C
1	X	1307	U
1	X	1313	U
1	X	1314	A
1	X	1315	A
1	X	1319	C
1	X	1334	A
1	X	1339	U
1	X	1341	G
1	X	1342	U
1	X	1358	C
1	X	1365	U
1	X	1378	A
1	X	1381	G
1	X	1392	U

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Mol	Chain	Res	Type
1	X	1399	C
1	X	1404	C
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	1441	A
1	X	1442	C
1	X	1443	G
1	X	1451	C
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	1473	U
1	X	1474	A
1	X	1475	U
1	X	1476	G
1	X	1482	U
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	1509	A
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	1531	C
1	X	1532	A
1	X	1533	G

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Mol	Chain	Res	Type
1	X	1545	G
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	1583	A
1	X	1584	G
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	1613	G
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	1648	C
1	X	1657	A
1	X	1665	C
1	X	1669	A
1	X	1691	G
1	X	1710	U
1	X	1711	C
1	X	1712	G
1	X	1713	G
1	X	1716	G
1	X	1717	A
1	X	1732	U
1	X	1733	U
1	X	1734	C
1	X	1747	G

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Mol	Chain	Res	Type
1	X	1754	G
1	X	1755	G
1	X	1764	A
1	X	1773	C
1	X	1776	A
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1799	A
1	X	1806	G
1	X	1807	A
1	X	1808	C
1	X	1812	U
1	X	1813	A
1	X	1820	G
1	X	1821	A
1	X	1825	C
1	X	1831	G
1	X	1840	A
1	X	1850	G
1	X	1861	G
1	X	1863	U
1	X	1867	A
1	X	1874	G
1	X	1882	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	1920	A
1	X	1921	A
1	X	1923	U
1	X	1939	U
1	X	1943	A
1	X	1947	G
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G

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Mol	Chain	Res	Type
1	X	1958	G
1	X	1963	G
1	X	1964	A
1	X	1965	U
1	X	1975	G
1	X	1976	U
1	X	1980	A
1	X	2006	G
1	X	2010	G
1	X	2014	A
1	X	2015	G
1	X	2018	G
1	X	2019	C
1	X	2026	C
1	X	2035	G
1	X	2038	C
1	X	2039	G
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2076	G
1	X	2079	A
1	X	2088	U
1	X	2089	C
1	X	2171	U
1	X	2180	U
1	X	2181	A
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2195	C
1	X	2196	U
1	X	2197	U
1	X	2198	U
1	X	2199	C
1	X	2204	A
1	X	2205	C
1	X	2217	G
1	X	2218	G
1	X	2222	U
1	X	2247	A

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Mol	Chain	Res	Type
1	X	2262	C
1	X	2265	A
1	X	2266	A
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	2291	U
1	X	2294	U
1	X	2295	C
1	X	2298	U
1	X	2299	A
1	X	2300	G
1	X	2301	A
1	X	2306	A
1	X	2313	G
1	X	2314	A
1	X	2315	A
1	X	2324	G
1	X	2325	A
1	X	2326	C
1	X	2329	C
1	X	2339	A
1	X	2351	G
1	X	2355	A
1	X	2358	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2370	G
1	X	2371	A
1	X	2375	G
1	X	2381	A
1	X	2382	C
1	X	2385	U
1	X	2389	G
1	X	2396	C
1	X	2401	A
1	X	2402	U
1	X	2404	A

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Mol	Chain	Res	Type
1	X	2405	A
1	X	2408	G
1	X	2409	A
1	X	2410	U
1	X	2420	C
1	X	2426	G
1	X	2427	A
1	X	2448	A
1	X	2449	G
1	X	2452	U
1	X	2455	A
1	X	2463	G
1	X	2470	U
1	X	2475	C
1	X	2477	C
1	X	2480	C
1	X	2481	G
1	X	2482	A
1	X	2483	U
1	X	2484	G
1	X	2485	U
1	X	2498	U
1	X	2499	C
1	X	2501	U
1	X	2504	G
1	X	2508	G
1	X	2514	G
1	X	2543	A
1	X	2545	A
1	X	2546	G
1	X	2548	G
1	X	2552	C
1	X	2553	G
1	X	2557	G
1	X	2561	G
1	X	2565	C
1	X	2580	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2589	C
1	X	2591	C

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Mol	Chain	Res	Type
1	X	2594	U
1	X	2600	A
1	X	2609	G
1	X	2611	A
1	X	2613	A
1	X	2615	U
1	X	2620	G
1	X	2633	A
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	2705	A
1	X	2706	U
1	X	2707	G
1	X	2713	A
1	X	2728	A
1	X	2731	G
1	X	2732	C
1	X	2736	U
1	X	2737	A
1	X	2738	A
1	X	2744	A
1	X	2745	A
1	X	2758	A
1	X	2759	U
1	X	2770	A
1	X	2771	C
1	X	2774	U
1	X	2775	U
1	X	2776	U
1	X	2777	A
1	X	2778	U
1	X	2779	C
1	X	2780	A
1	X	2782	G
1	X	2795	A
1	X	2796	A
1	X	2808	U

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Mol	Chain	Res	Type
1	X	2810	A
1	X	2811	G
1	X	2824	C
1	X	2825	A
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	2859	U
1	X	2868	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	39	C
2	Y	42	U
2	Y	43	G
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	53	G
2	Y	54	U
2	Y	56	G
2	Y	58	G
2	Y	59	A
2	Y	69	G
2	Y	75	A
2	Y	76	U
2	Y	99	G
2	Y	102	A
2	Y	108	G
2	Y	112	A
2	Y	115	G
2	Y	123	U

All (243) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	3	U
1	X	13	A
1	X	33	C
1	X	48	A
1	X	50	G
1	X	62	U
1	X	70	A
1	X	71	A
1	X	74	G
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	124	A
1	X	154	U
1	X	176	A
1	X	190	A
1	X	198	A
1	X	199	A
1	X	242	A
1	X	312	G
1	X	321	A
1	X	322	A
1	X	328	A
1	X	332	C
1	X	334	G
1	X	341	A
1	X	342	G
1	X	343	A
1	X	396	U
1	X	399	G
1	X	416	U
1	X	417	C
1	X	418	C
1	X	458	G
1	X	466	A
1	X	467	U
1	X	469	G
1	X	490	A
1	X	504	G

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Mol	Chain	Res	Type
1	X	513	A
1	X	522	G
1	X	537	C
1	X	539	A
1	X	542	A
1	X	553	C
1	X	554	U
1	X	557	U
1	X	558	G
1	X	559	C
1	X	580	A
1	X	583	C
1	X	648	A
1	X	655	A
1	X	664	C
1	X	668	A
1	X	672	C
1	X	682	G
1	X	683	A
1	X	698	A
1	X	751	G
1	X	758	G
1	X	759	C
1	X	761	G
1	X	777	A
1	X	780	U
1	X	788	G
1	X	789	G
1	X	796	A
1	X	802	A
1	X	803	C
1	X	806	A
1	X	813	A
1	X	814	G
1	X	824	U
1	X	841	G
1	X	842	A
1	X	858	G
1	X	859	U
1	X	872	G
1	X	878	C
1	X	879	A

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Mol	Chain	Res	Type
1	X	939	C
1	X	940	G
1	X	955	G
1	X	969	U
1	X	972	C
1	X	994	A
1	X	1000	G
1	X	1031	C
1	X	1033	G
1	X	1037	U
1	X	1053	G
1	X	1055	A
1	X	1056	U
1	X	1072	U
1	X	1081	A
1	X	1086	C
1	X	1096	A
1	X	1099	A
1	X	1120	C
1	X	1121	G
1	X	1139	A
1	X	1141	U
1	X	1152	C
1	X	1154	A
1	X	1182	U
1	X	1186	G
1	X	1191	G
1	X	1194	U
1	X	1223	G
1	X	1233	A
1	X	1249	G
1	X	1288	A
1	X	1299	A
1	X	1313	U
1	X	1314	A
1	X	1353	A
1	X	1357	U
1	X	1378	A
1	X	1409	U
1	X	1410	U
1	X	1412	C
1	X	1432	G

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Mol	Chain	Res	Type
1	X	1433	A
1	X	1441	A
1	X	1442	C
1	X	1459	U
1	X	1473	U
1	X	1475	U
1	X	1496	G
1	X	1505	U
1	X	1513	U
1	X	1531	C
1	X	1541	G
1	X	1552	C
1	X	1561	A
1	X	1562	G
1	X	1574	A
1	X	1575	C
1	X	1581	C
1	X	1583	A
1	X	1601	U
1	X	1607	A
1	X	1618	U
1	X	1624	A
1	X	1625	A
1	X	1631	C
1	X	1680	U
1	X	1710	U
1	X	1711	C
1	X	1716	G
1	X	1732	U
1	X	1775	A
1	X	1777	A
1	X	1790	G
1	X	1791	C
1	X	1799	A
1	X	1800	A
1	X	1807	A
1	X	1810	U
1	X	1811	A
1	X	1812	U
1	X	1820	G
1	X	1865	C
1	X	1872	A

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Mol	Chain	Res	Type
1	X	1882	G
1	X	1883	A
1	X	1909	U
1	X	1920	A
1	X	1921	A
1	X	1938	U
1	X	1953	A
1	X	1963	G
1	X	1975	G
1	X	1980	A
1	X	2014	A
1	X	2018	G
1	X	2075	U
1	X	2083	G
1	X	2088	U
1	X	2180	U
1	X	2181	A
1	X	2189	A
1	X	2198	U
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	2298	U
1	X	2299	A
1	X	2305	C
1	X	2312	A
1	X	2314	A
1	X	2324	G
1	X	2354	G
1	X	2361	G
1	X	2370	G
1	X	2381	A
1	X	2401	A
1	X	2404	A
1	X	2409	A
1	X	2447	G
1	X	2477	C
1	X	2482	A
1	X	2497	A

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Mol	Chain	Res	Type
1	X	2498	U
1	X	2560	G
1	X	2564	U
1	X	2580	C
1	X	2608	A
1	X	2615	U
1	X	2624	G
1	X	2660	C
1	X	2669	C
1	X	2691	C
1	X	2705	A
1	X	2706	U
1	X	2731	G
1	X	2736	U
1	X	2744	A
1	X	2758	A
1	X	2769	C
1	X	2770	A
1	X	2778	U
1	X	2807	U
1	X	2808	U
1	X	2810	A
1	X	2824	C
1	X	2846	G
1	X	2848	A
1	X	2854	G
1	X	2867	G
2	Y	26	G
2	Y	46	G
2	Y	54	U
2	Y	58	G
2	Y	86	A

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	1F3	X	2931	-	62,64,64	1.25	7 (11%)	83,96,96	1.82	17 (20%)

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	1F3	X	2931	-	-	8/78/119/119	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2931	1F3	C48-C47	-3.93	1.51	1.54
32	X	2931	1F3	C50-C49	3.60	1.50	1.34
32	X	2931	1F3	C50-N45	3.14	1.44	1.38
32	X	2931	1F3	O17-C5	-3.04	1.43	1.47
32	X	2931	1F3	C41-N40	2.42	1.37	1.33
32	X	2931	1F3	C47-N45	-2.39	1.43	1.47
32	X	2931	1F3	C51-C47	-2.03	1.48	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	X	2931	1F3	C59-C58-N57	-5.64	106.72	114.98
32	X	2931	1F3	C23-C6-C5	-4.94	108.42	115.23
32	X	2931	1F3	C28-O20-C8	-4.85	107.83	116.25
32	X	2931	1F3	O60-C58-N57	4.00	128.31	123.04
32	X	2931	1F3	C47-N45-C50	3.30	113.23	109.75
32	X	2931	1F3	C48-C47-C51	-3.20	108.03	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	X	2931	1F3	O29-C30-C38	-3.01	100.49	106.88
32	X	2931	1F3	C27-C12-C13	-2.93	106.28	112.92
32	X	2931	1F3	C24-C5-C4	-2.72	112.59	116.42
32	X	2931	1F3	C30-C31-C32	-2.55	105.99	110.46
32	X	2931	1F3	C47-C48-C49	2.32	107.55	103.02
32	X	2931	1F3	C52-C51-C47	-2.29	116.42	120.76
32	X	2931	1F3	O10-C6-C23	2.22	111.63	107.40
32	X	2931	1F3	C9-C7-C2	2.21	119.85	116.11
32	X	2931	1F3	O43-C13-C12	-2.21	103.66	107.55
32	X	2931	1F3	O10-C11-O26	2.19	128.02	123.94
32	X	2931	1F3	C16-C1-C3	-2.11	104.41	108.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2931	1F3	C59-C58-N57-C54
32	X	2931	1F3	O60-C58-N57-C54
32	X	2931	1F3	C16-C1-C4-N40
32	X	2931	1F3	O20-C8-C9-C7
32	X	2931	1F3	C3-C2-C7-C9
32	X	2931	1F3	C14-C8-C9-C7
32	X	2931	1F3	O20-C8-C9-C22
32	X	2931	1F3	C16-C1-C4-C5

There are no ring outliers.

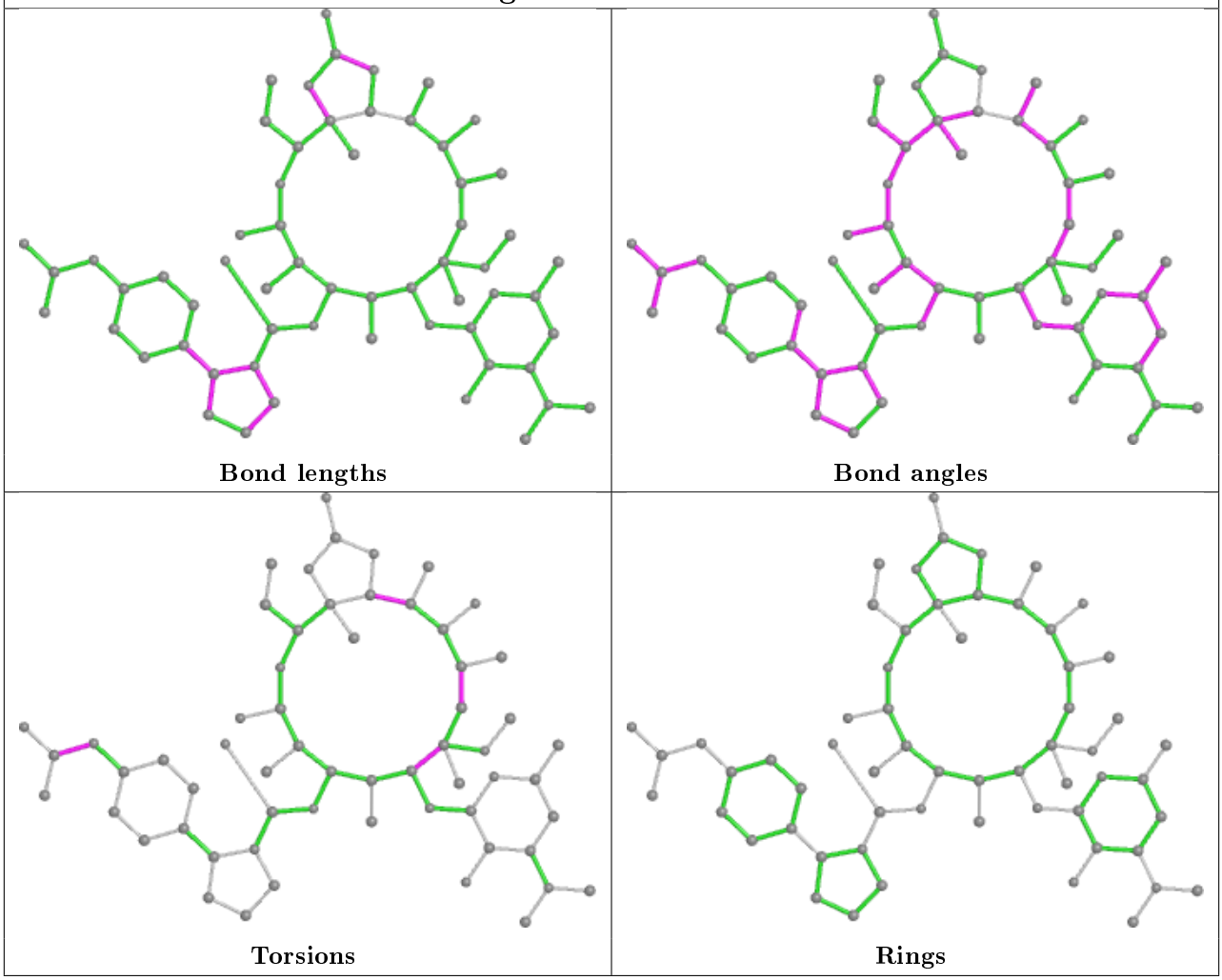
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2931	1F3	2	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 then 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.

Ligand 1F3 X 2931



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.21	69 (2%) 56 40	43, 87, 194, 279	0
2	Y	122/123 (99%)	-0.14	2 (1%) 72 59	82, 129, 165, 187	0
3	A	240/274 (87%)	0.03	5 (2%) 63 49	63, 107, 137, 156	0
4	B	205/211 (97%)	-0.35	3 (1%) 73 61	38, 68, 99, 145	0
5	C	197/205 (96%)	0.13	14 (7%) 16 9	55, 107, 150, 178	0
6	D	177/180 (98%)	0.42	14 (7%) 12 6	148, 178, 210, 216	0
7	E	171/185 (92%)	-0.16	4 (2%) 60 47	98, 139, 178, 188	0
8	F	71/144 (49%)	2.66	36 (50%) 0 0	221, 234, 251, 259	0
9	G	142/174 (81%)	0.05	8 (5%) 24 13	65, 89, 137, 149	0
10	H	134/134 (100%)	-0.51	0 100 100	49, 62, 88, 110	0
11	I	141/156 (90%)	0.74	22 (15%) 2 1	54, 120, 171, 195	0
12	J	136/141 (96%)	0.02	5 (3%) 41 26	83, 106, 147, 172	0
13	K	113/116 (97%)	-0.51	0 100 100	37, 53, 71, 99	0
14	L	104/114 (91%)	0.26	5 (4%) 30 18	91, 122, 149, 166	0
15	M	108/166 (65%)	-0.53	0 100 100	44, 64, 106, 128	0
16	N	117/118 (99%)	-0.30	2 (1%) 70 57	54, 86, 124, 152	0
17	O	94/100 (94%)	-0.16	3 (3%) 47 31	67, 106, 146, 160	0
18	P	127/134 (94%)	-0.50	0 100 100	48, 64, 103, 143	0
19	Q	93/95 (97%)	0.07	5 (5%) 25 14	69, 101, 156, 193	0
20	R	110/115 (95%)	0.37	12 (10%) 5 3	84, 113, 170, 173	0
21	S	175/237 (73%)	0.27	12 (6%) 16 9	119, 154, 178, 190	0
22	T	84/91 (92%)	0.77	16 (19%) 1 1	72, 103, 176, 195	0
23	U	72/81 (88%)	0.53	5 (6%) 16 9	86, 122, 146, 182	0
24	V	66/67 (98%)	0.74	8 (12%) 4 2	88, 128, 213, 230	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	55/55 (100%)	-0.31	0 100 100	76, 96, 123, 161	0
26	Z	58/60 (96%)	-0.27	2 (3%) 45 29	47, 64, 96, 108	0
27	1	53/55 (96%)	0.84	9 (16%) 1 1	6, 28, 62, 73	0
28	2	46/47 (97%)	2.80	29 (63%) 0 0	3, 10, 27, 42	0
29	3	63/66 (95%)	2.07	26 (41%) 0 0	3, 18, 41, 84	0
30	4	37/37 (100%)	7.99	36 (97%) 0 0	191, 239, 247, 252	0
All	All	5997/6561 (91%)	0.05	352 (5%) 22 13	3, 96, 193, 279	0

All (352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	25	VAL	20.1
30	4	16	VAL	17.6
24	V	1	MET	16.3
8	F	114	ASP	15.7
30	4	29	ASN	15.4
30	4	17	VAL	14.3
30	4	24	LEU	13.5
30	4	6	SER	12.5
22	T	9	SER	12.3
30	4	28	SER	12.0
30	4	11	CYS	11.8
1	X	731	A	10.9
30	4	34	GLN	10.6
27	1	4	ASP	10.6
23	U	27	ASP	10.3
24	V	3	PRO	10.2
30	4	32	HIS	10.1
8	F	137	THR	9.9
30	4	7	VAL	9.9
30	4	23	VAL	9.7
30	4	10	MET	8.9
11	I	8	PRO	8.7
29	3	33	ASN	8.6
30	4	20	HIS	8.5
30	4	36	GLN	8.1
2	Y	123	U	7.9
1	X	1089	C	7.7
30	4	21	GLY	7.7
30	4	35	ARG	7.6

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Mol	Chain	Res	Type	RSRZ
30	4	14	CYS	7.6
1	X	1086	C	7.5
3	A	203	ASN	7.5
19	Q	64	ARG	7.5
22	T	6	GLY	7.4
24	V	2	LYS	7.4
22	T	10	SER	7.3
30	4	27	CYS	7.2
23	U	28	GLY	7.2
8	F	113	PRO	7.1
11	I	9	THR	7.1
29	3	60	LEU	7.1
8	F	136	VAL	6.8
1	X	1085	G	6.7
11	I	5	ASP	6.7
6	D	43	SER	6.6
11	I	4	HIS	6.6
30	4	15	LYS	6.6
30	4	22	ARG	6.5
12	J	84	MET	6.4
24	V	4	SER	6.3
30	4	19	ARG	6.3
30	4	26	ILE	6.3
8	F	97	GLY	6.3
30	4	5	SER	6.3
8	F	98	LYS	6.2
28	2	9	ASN	6.2
9	G	156	HIS	6.1
26	Z	2	ALA	6.1
29	3	11	LYS	6.1
5	C	165	SER	6.0
9	G	155	THR	5.9
22	T	8	GLY	5.9
20	R	100	ASP	5.7
20	R	99	VAL	5.7
27	1	7	ARG	5.7
11	I	6	LEU	5.7
1	X	1079	G	5.6
5	C	47	THR	5.6
22	T	7	VAL	5.6
28	2	27	GLY	5.6
1	X	1069	G	5.6

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Mol	Chain	Res	Type	RSRZ
30	4	13	ASN	5.5
29	3	27	SER	5.5
3	A	250	TRP	5.4
29	3	31	HIS	5.4
1	X	1524	C	5.4
30	4	12	ASP	5.4
1	X	1186	G	5.4
11	I	52	GLY	5.2
1	X	1095	A	5.2
28	2	4	THR	5.2
20	R	94	VAL	5.1
11	I	29	THR	5.1
8	F	125	ASN	5.1
1	X	248	A	5.1
27	1	24	THR	5.0
1	X	730	C	5.0
11	I	63	ARG	5.0
8	F	84	ILE	5.0
30	4	4	ARG	5.0
30	4	33	LYS	4.8
28	2	36	ALA	4.8
28	2	8	ASN	4.8
28	2	7	PRO	4.8
30	4	30	VAL	4.7
20	R	102	LYS	4.7
1	X	1091	C	4.7
30	4	1	MET	4.7
29	3	30	ARG	4.7
2	Y	2	C	4.7
6	D	23	SER	4.7
28	2	24	THR	4.6
22	T	4	LYS	4.5
6	D	42	SER	4.5
8	F	131	ALA	4.5
9	G	97	ASP	4.4
28	2	34	ARG	4.4
28	2	32	ALA	4.4
28	2	11	LYS	4.3
1	X	1114	A	4.3
5	C	19	LEU	4.3
8	F	123	ALA	4.3
1	X	1080	A	4.3

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Mol	Chain	Res	Type	RSRZ
27	1	41	ASP	4.3
30	4	9	LYS	4.3
24	V	6	MET	4.3
29	3	42	ARG	4.2
1	X	2088	U	4.2
22	T	15	ASP	4.1
22	T	3	HIS	4.1
29	3	39	ASP	4.1
1	X	1077	U	4.1
8	F	126	THR	4.1
1	X	1068	A	4.1
8	F	121	GLU	4.0
8	F	144	ALA	4.0
21	S	124	ALA	4.0
24	V	11	ALA	4.0
1	X	1104	G	4.0
1	X	2089	C	4.0
1	X	1078	A	4.0
28	2	6	GLN	4.0
1	X	1090	C	4.0
1	X	1106	A	4.0
22	T	5	LYS	3.9
5	C	123	PHE	3.9
28	2	29	ASN	3.9
1	X	1523	A	3.9
1	X	2776	U	3.9
11	I	7	LYS	3.8
27	1	43	VAL	3.8
8	F	119	SER	3.8
12	J	140	GLU	3.8
1	X	1187	A	3.8
28	2	30	ILE	3.8
1	X	1525	A	3.8
8	F	92	ASN	3.7
29	3	7	HIS	3.7
8	F	111	LYS	3.7
29	3	34	THR	3.7
21	S	15	ASP	3.7
1	X	891	A	3.6
5	C	21	GLU	3.6
6	D	145	MET	3.6
8	F	96	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
23	U	16	ASN	3.6
8	F	133	SER	3.6
8	F	107	ILE	3.6
21	S	91	PRO	3.6
1	X	2778	U	3.6
19	Q	69	ILE	3.6
1	X	361	G	3.6
1	X	728	G	3.5
11	I	30	ALA	3.5
7	E	5	GLY	3.5
8	F	112	MET	3.5
29	3	10	ALA	3.5
23	U	47	HIS	3.5
30	4	8	LYS	3.5
1	X	1188	A	3.5
4	B	205	SER	3.5
30	4	3	VAL	3.5
17	O	39	PHE	3.5
1	X	1084	A	3.4
6	D	134	GLU	3.4
29	3	28	GLY	3.4
11	I	10	PRO	3.4
29	3	6	THR	3.4
1	X	1067	G	3.3
4	B	94	ASP	3.3
8	F	115	LEU	3.3
28	2	5	TYR	3.3
5	C	44	SER	3.3
21	S	12	GLN	3.3
1	X	729	A	3.3
8	F	110	THR	3.3
28	2	23	LYS	3.3
22	T	17	ASN	3.3
6	D	147	ASP	3.3
20	R	101	GLY	3.2
5	C	20	PRO	3.2
6	D	94	GLU	3.2
28	2	2	LYS	3.2
6	D	76	ASN	3.2
3	A	249	PRO	3.2
21	S	24	TYR	3.2
28	2	22	MET	3.1

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Mol	Chain	Res	Type	RSRZ
6	D	144	ASP	3.1
1	X	2280	A	3.1
3	A	219	PRO	3.1
28	2	21	ARG	3.1
8	F	122	ALA	3.1
1	X	2777	A	3.1
1	X	1189	G	3.1
29	3	5	LYS	3.1
29	3	40	GLU	3.1
14	L	34	SER	3.0
17	O	41	GLY	3.0
20	R	58	VAL	3.0
24	V	36	GLN	3.0
8	F	93	LYS	3.0
11	I	50	GLU	3.0
28	2	1	MET	3.0
8	F	127	VAL	3.0
11	I	48	PHE	3.0
21	S	14	LEU	2.9
28	2	25	LYS	2.9
6	D	146	VAL	2.9
1	X	1098	G	2.9
5	C	91	TYR	2.9
14	L	64	LYS	2.9
27	1	25	THR	2.9
29	3	36	LYS	2.8
29	3	2	PRO	2.8
11	I	82	ASP	2.8
6	D	11	GLN	2.8
9	G	103	TYR	2.8
30	4	37	GLY	2.8
8	F	94	ALA	2.8
8	F	129	GLY	2.8
21	S	60	GLU	2.8
11	I	33	GLY	2.8
1	X	665	A	2.7
11	I	54	SER	2.7
29	3	8	LYS	2.7
11	I	36	GLY	2.7
8	F	99	LEU	2.7
29	3	37	SER	2.7
8	F	128	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	X	1734	C	2.7
1	X	1093	U	2.7
22	T	85	GLN	2.7
6	D	37	ASN	2.7
27	1	3	LYS	2.7
28	2	10	ARG	2.7
4	B	135	HIS	2.7
1	X	1088	A	2.7
1	X	1913	G	2.6
1	X	1072	U	2.6
28	2	41	GLN	2.6
20	R	82	ALA	2.6
8	F	118	GLY	2.6
8	F	108	ALA	2.6
8	F	143	ASN	2.6
6	D	113	ASP	2.6
9	G	37	ASP	2.6
28	2	26	SER	2.6
8	F	83	GLY	2.6
26	Z	3	LYS	2.6
8	F	120	VAL	2.6
12	J	85	GLY	2.6
20	R	103	LYS	2.6
24	V	12	THR	2.5
29	3	32	GLN	2.5
29	3	17	THR	2.5
9	G	162	LYS	2.5
1	X	1551	U	2.5
1	X	1115	C	2.5
1	X	1076	U	2.5
9	G	129	HIS	2.4
29	3	47	GLY	2.4
9	G	106	TYR	2.4
1	X	1109	A	2.4
30	4	2	LYS	2.4
1	X	1094	C	2.4
14	L	97	HIS	2.4
7	E	46	ASP	2.4
22	T	11	LYS	2.4
17	O	5	ILE	2.4
11	I	53	ARG	2.4
5	C	48	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	X	2172	U	2.4
1	X	2775	U	2.4
28	2	20	ALA	2.4
30	4	18	ARG	2.3
1	X	1102	G	2.3
29	3	18	GLY	2.3
1	X	727	U	2.3
5	C	189	ASP	2.3
8	F	102	ASP	2.3
20	R	93	ARG	2.3
12	J	90	ALA	2.3
1	X	435	A	2.3
1	X	1037	U	2.3
8	F	91	PRO	2.3
21	S	93	GLU	2.3
1	X	1120	C	2.3
1	X	1841	G	2.3
28	2	3	ARG	2.3
29	3	4	MET	2.3
20	R	61	SER	2.3
5	C	198	GLU	2.3
27	1	27	ASN	2.3
11	I	67	ASN	2.2
5	C	172	VAL	2.2
21	S	123	VAL	2.2
19	Q	72	ARG	2.2
28	2	31	LEU	2.2
1	X	732	G	2.2
5	C	193	LEU	2.2
11	I	100	ARG	2.2
20	R	77	HIS	2.2
3	A	85	ASP	2.2
1	X	1057	A	2.2
1	X	2581	A	2.2
23	U	26	ALA	2.2
1	X	1553	G	2.2
22	T	71	ASN	2.2
22	T	84	ALA	2.2
1	X	1070	G	2.2
1	X	304	A	2.2
1	X	1092	U	2.1
19	Q	65	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	2170	C	2.1
27	1	44	ALA	2.1
1	X	2174	G	2.1
22	T	2	ALA	2.1
14	L	36	LYS	2.1
28	2	16	HIS	2.1
28	2	28	ARG	2.1
6	D	153	ASP	2.1
1	X	1087	C	2.1
7	E	58	ALA	2.1
16	N	94	VAL	2.1
20	R	63	THR	2.1
7	E	29	PRO	2.1
21	S	86	VAL	2.1
12	J	14	PHE	2.0
19	Q	63	LYS	2.0
29	3	61	MET	2.1
1	X	1101	U	2.0
1	X	358	C	2.0
21	S	10	PRO	2.0
28	2	19	ARG	2.0
11	I	56	LEU	2.0
14	L	53	ALA	2.0
22	T	12	ASN	2.0
5	C	197	GLU	2.0
21	S	92	VAL	2.0
11	I	60	LEU	2.0
29	3	38	GLY	2.0
16	N	92	ARG	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)

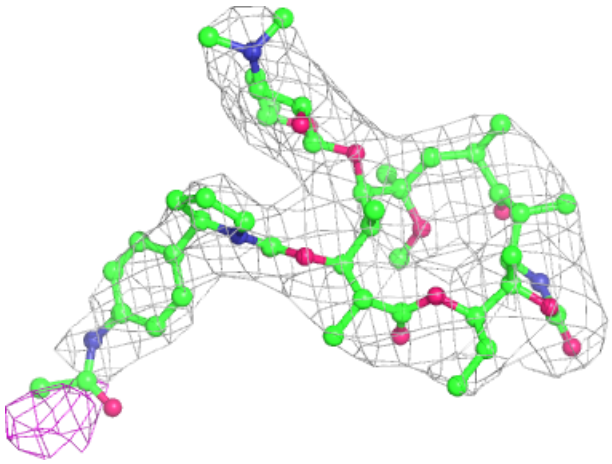
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

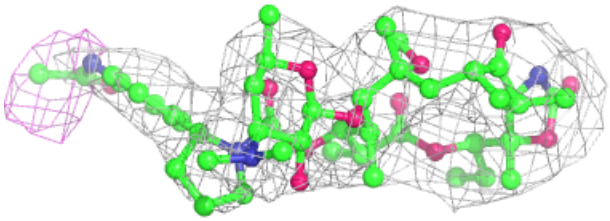
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	2904	1/1	0.56	0.55	90,90,90,90	0
31	MG	X	2922	1/1	0.65	0.87	81,81,81,81	0
31	MG	X	2905	1/1	0.70	0.54	104,104,104,104	0
31	MG	Y	203	1/1	0.75	0.49	87,87,87,87	0
31	MG	X	2910	1/1	0.78	0.18	85,85,85,85	0
31	MG	Y	205	1/1	0.79	0.34	77,77,77,77	0
31	MG	X	2929	1/1	0.80	0.36	77,77,77,77	0
31	MG	X	2913	1/1	0.81	0.56	66,66,66,66	0
31	MG	X	2901	1/1	0.83	0.39	110,110,110,110	0
31	MG	Y	201	1/1	0.84	0.50	82,82,82,82	0
31	MG	X	2927	1/1	0.84	0.48	106,106,106,106	0
31	MG	X	2930	1/1	0.86	0.99	71,71,71,71	0
31	MG	X	2906	1/1	0.87	0.40	79,79,79,79	0
31	MG	X	2908	1/1	0.89	0.51	49,49,49,49	0
31	MG	X	2912	1/1	0.90	0.29	60,60,60,60	0
31	MG	X	2916	1/1	0.91	0.56	53,53,53,53	0
31	MG	X	2926	1/1	0.93	1.00	56,56,56,56	0
31	MG	X	2925	1/1	0.94	0.46	39,39,39,39	0
31	MG	Y	204	1/1	0.95	0.19	67,67,67,67	0
31	MG	X	2909	1/1	0.95	1.00	37,37,37,37	0
31	MG	Y	202	1/1	0.95	0.48	54,54,54,54	0
31	MG	X	2919	1/1	0.95	0.57	56,56,56,56	0
31	MG	X	2903	1/1	0.96	0.13	82,82,82,82	0
31	MG	X	2914	1/1	0.96	0.59	51,51,51,51	0
32	1F3	X	2931	60/60	0.97	0.23	38,60,90,99	0
31	MG	X	2902	1/1	0.97	0.42	45,45,45,45	0
31	MG	X	2920	1/1	0.97	0.63	38,38,38,38	0
31	MG	X	2924	1/1	0.97	0.64	39,39,39,39	0
31	MG	X	2921	1/1	0.97	0.47	18,18,18,18	0
31	MG	X	2923	1/1	0.98	0.82	74,74,74,74	0
31	MG	X	2907	1/1	0.98	0.42	53,53,53,53	0
31	MG	X	2918	1/1	0.98	0.59	32,32,32,32	0
31	MG	X	2928	1/1	0.98	0.89	42,42,42,42	0
31	MG	X	2917	1/1	0.98	0.85	37,37,37,37	0
31	MG	X	2915	1/1	0.99	0.28	24,24,24,24	0
31	MG	X	2911	1/1	0.99	0.43	35,35,35,35	0

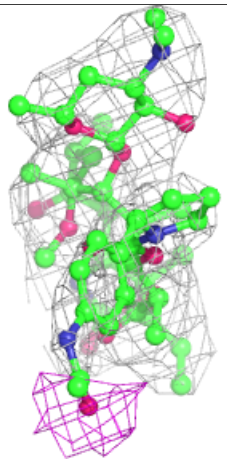
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1F3 X 2931:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers

There are no such residues in this entry.