Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 07:16 PM EDT

PDB ID	:	3PIO
Title	:	Crystal structure of the synergistic antibiotic pair lankamycin and lankacidin in complex with the large ribosomal subunit
Authors	:	Belousoff, M.J.; Shapira, T.; Bashan, A.; Zimmerman, E.; Arakawa, K.; Kinashi, H.; Rozenberg, H.; Yonath, A.
Deposited on	:	2010-11-07
Resolution	:	3.25 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

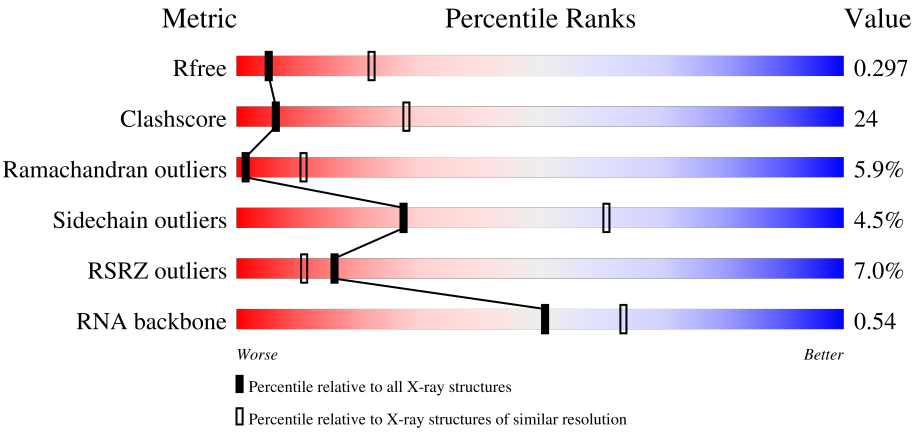
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.25 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)
RNA backbone	3102	1034 (3.58-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 32% 40% 18% • 8%
2	Y	123	2% 48% 41% 8% •
3	A	274	5% 42% 45% 5% 8%

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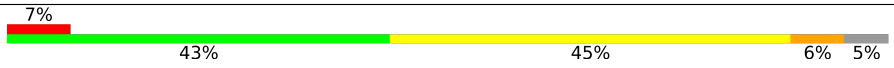
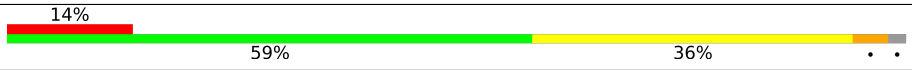
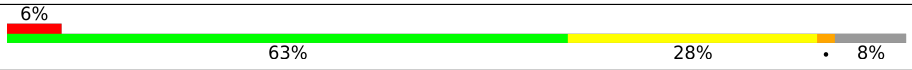
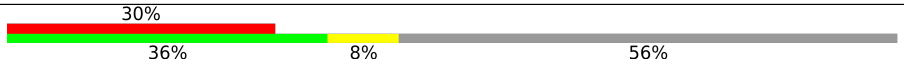
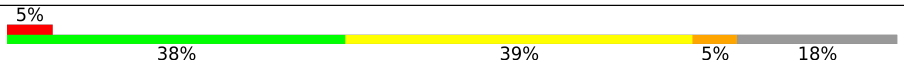
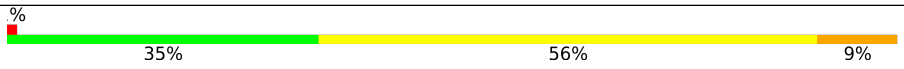
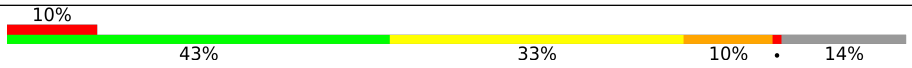
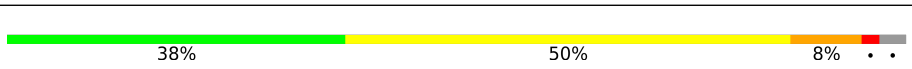
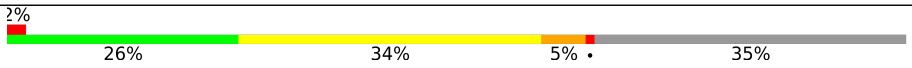
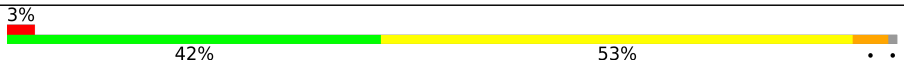
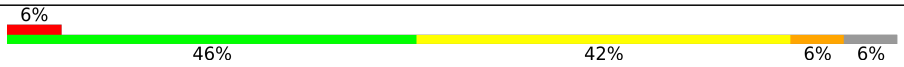
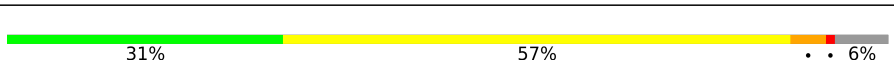
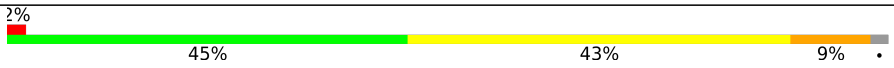
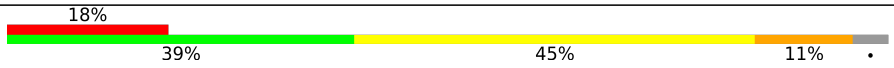
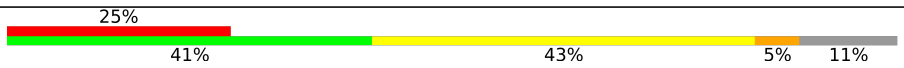
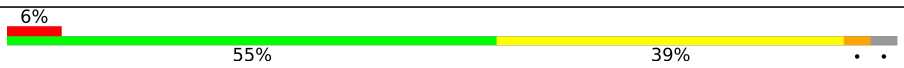
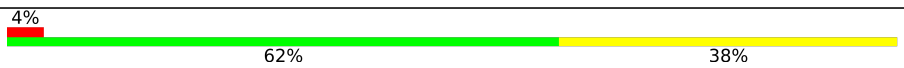
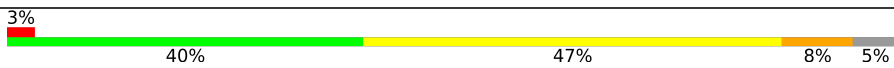
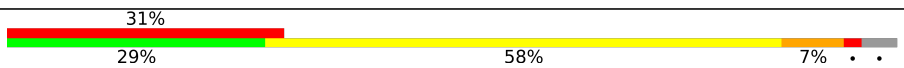
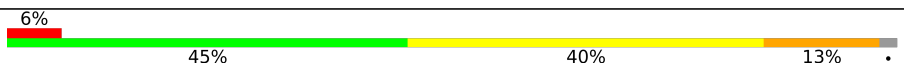
Mol	Chain	Length	Quality of chain
4	B	211	
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	

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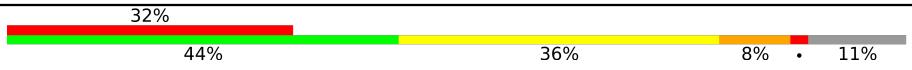
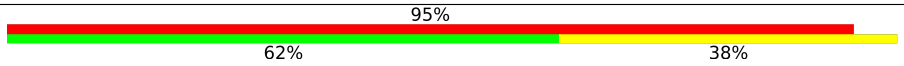
Mol	Chain	Length	Quality of chain
29	3	66	
30	4	37	

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
34	K	X	3074	-	-	-	X

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 84383 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 RIBOSOMAL 23S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	2657	57035	25441	10530	18408	2656	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	120	2561	1143	471	827	120	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	253	1920	1196	382	340	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	194	1481	920	284	275	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	63	Total	C	N	O	S	0	0	0
			451	280	82	86	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	134	Total	C	N	O	0	0	0
			1011	619	206	186			

- 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 779	C 476	N 161	O 142	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	126	Total 1004	C 633	N 197	O 172	S 2	0	0	0

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

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

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

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

- 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	74	Total	C	N	O	S	0	0	0
			556	351	107	97	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	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

- 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	57	Total	C	N	O	S	0	0	0
			452	278	93	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

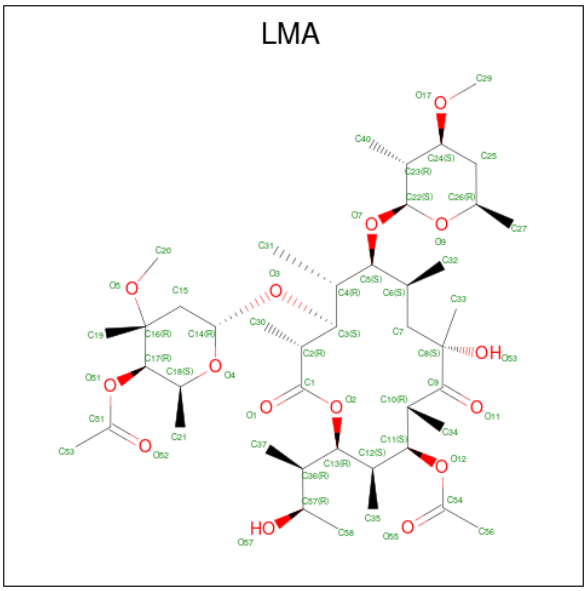
- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

- 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	0	0	0
			297	179	66	47	5			

- Molecule 31 is Lankamycin (three-letter code: LMA) (formula: $C_{43}H_{74}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	X	1	Total	C	O	0	0
			58	43	15		

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	151	Total	Mg	0	0
			151	151		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	Y	1	Total Mg 1 1	0	0
32	C	1	Total Mg 1 1	0	0
32	I	1	Total Mg 1 1	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	X	37	Total Na 37 37	0	0
33	Y	2	Total Na 2 2	0	0
33	A	1	Total Na 1 1	0	0
33	K	1	Total Na 1 1	0	0
33	Z	1	Total Na 1 1	0	0

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

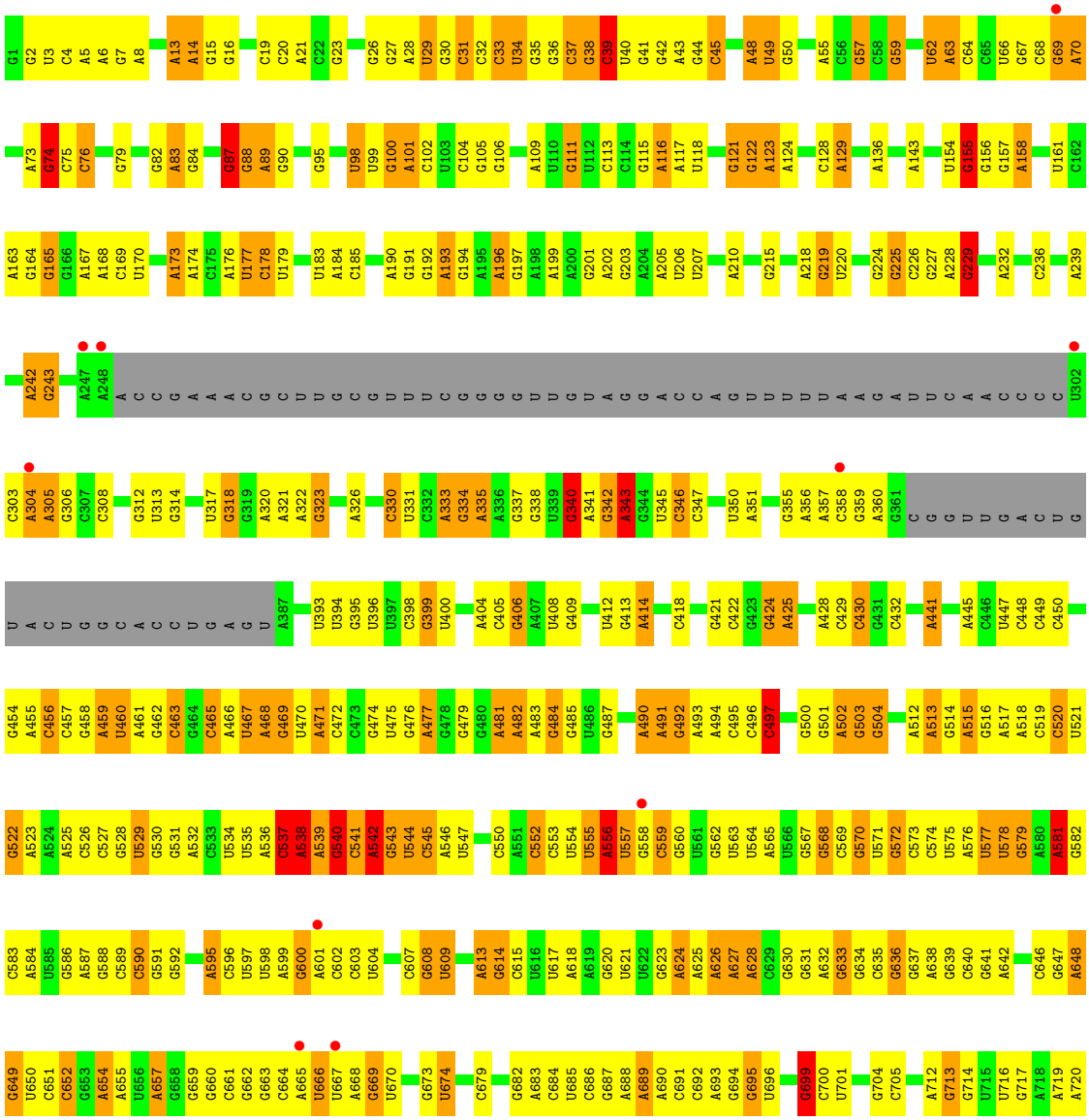
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	X	14	Total K 14 14	0	0
34	M	1	Total K 1 1	0	0

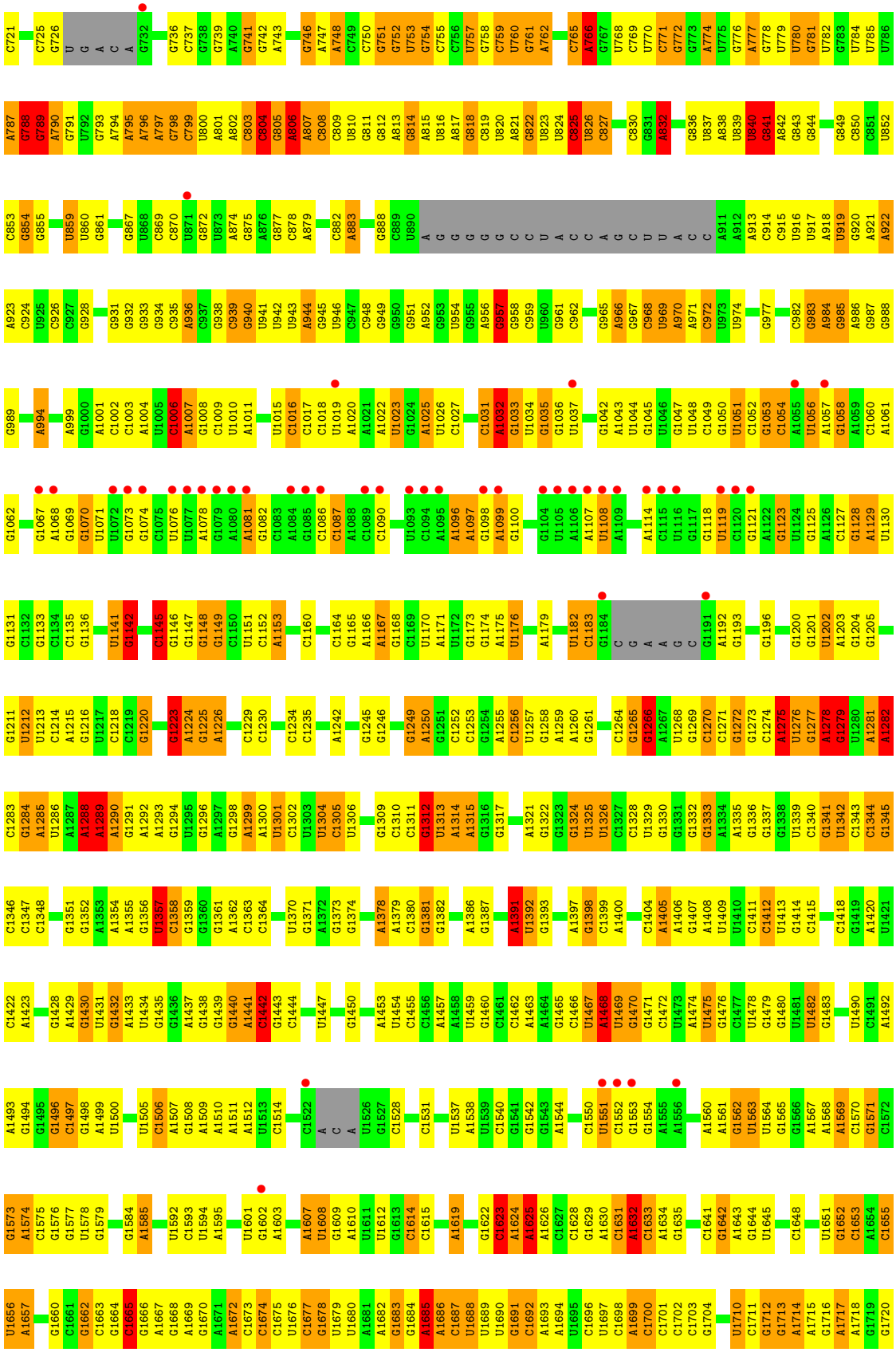
3 Residue-property plots (i)

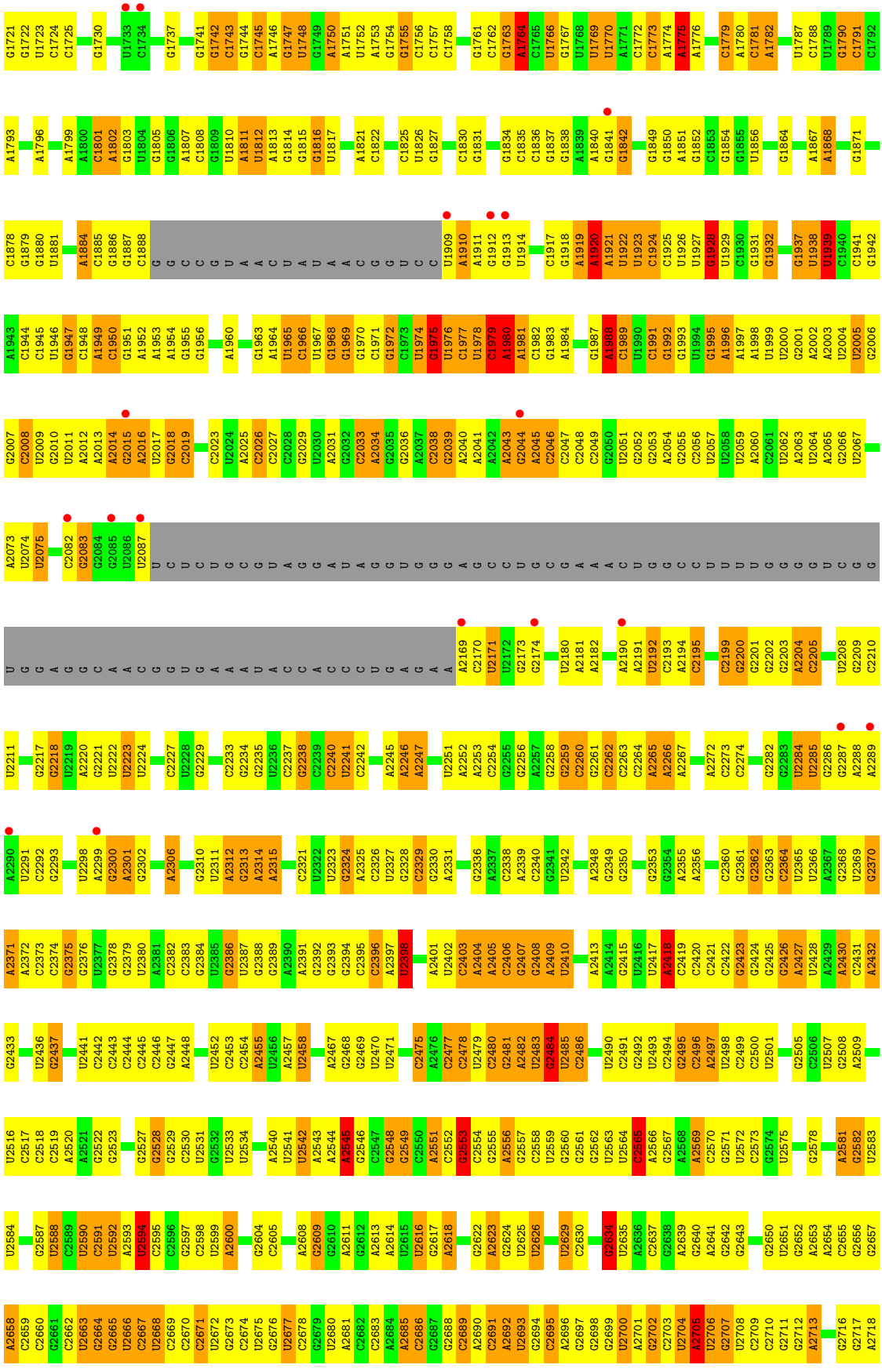
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

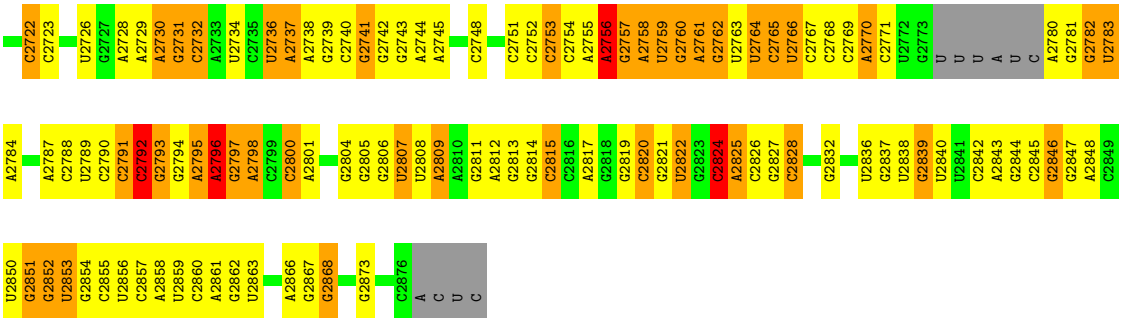
- Molecule 1: RIBOSOMAL 23S RNA

Chain X:



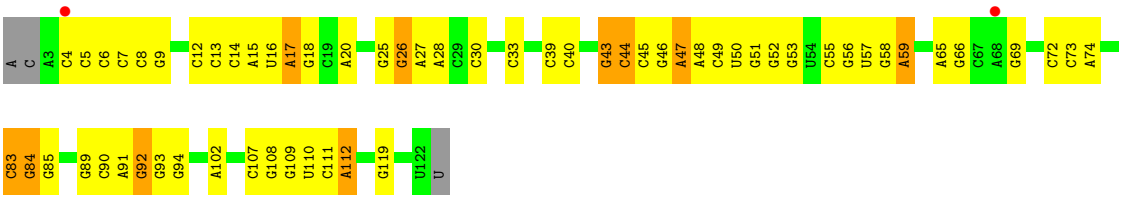






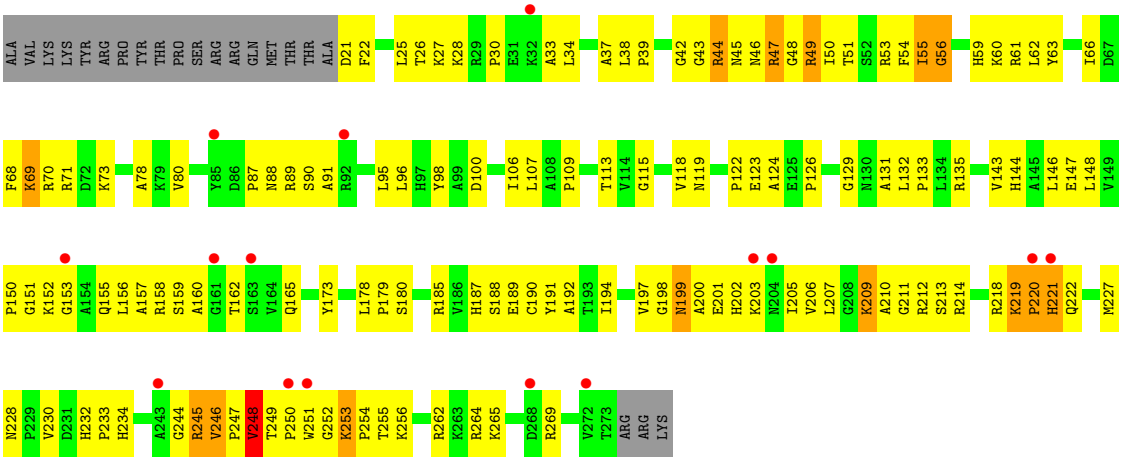
• Molecule 2: 5S ribosomal RNA

Chain Y:



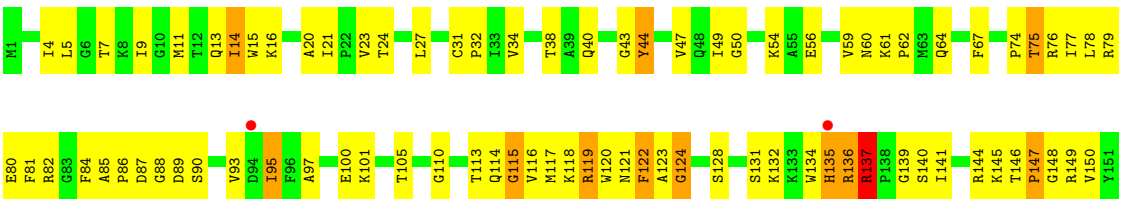
• Molecule 3: 50S ribosomal protein L2

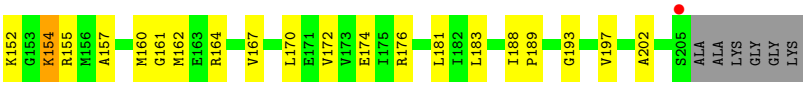
Chain A:



• Molecule 4: 50S ribosomal protein L3

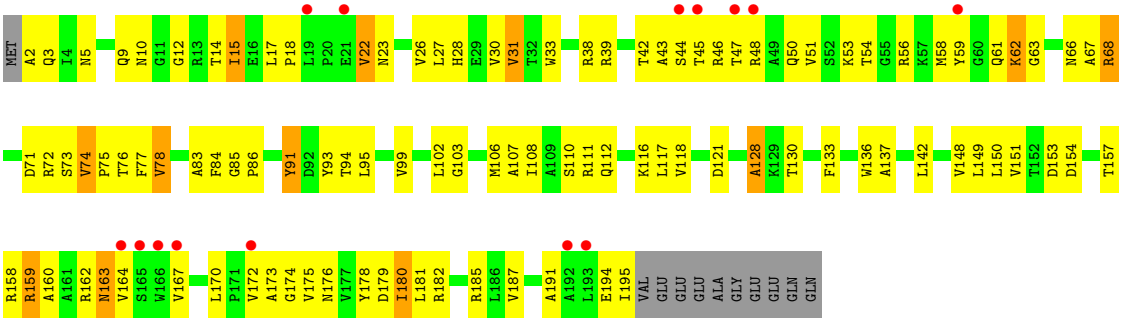
Chain B:





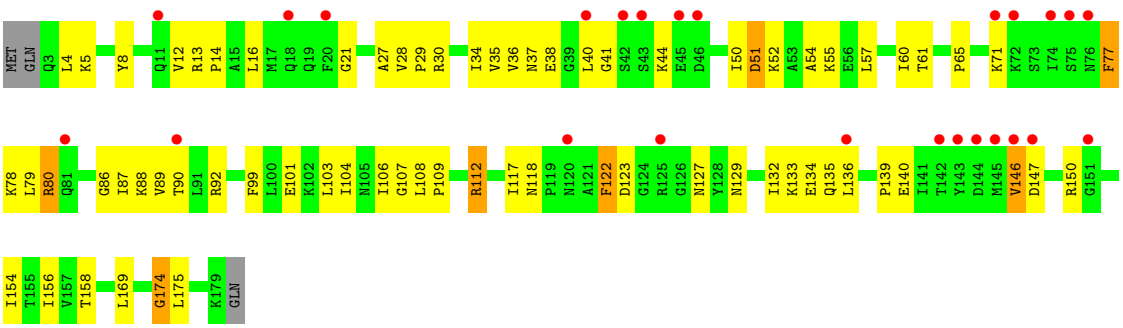
• Molecule 5: 50S ribosomal protein L4

Chain C:



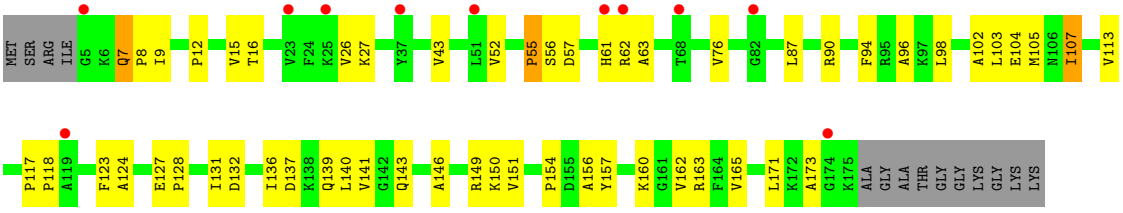
• Molecule 6: 50S ribosomal protein L5

Chain D:



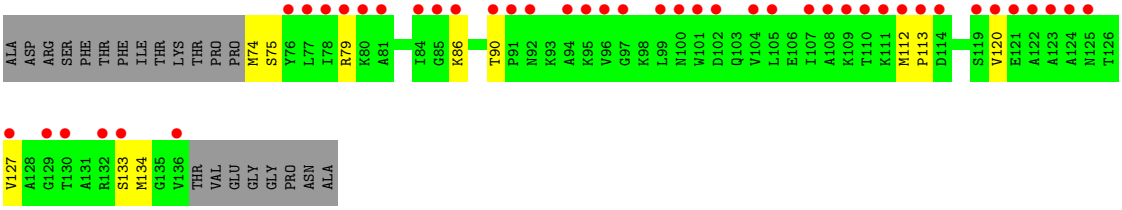
• Molecule 7: 50S ribosomal protein L6

Chain E:



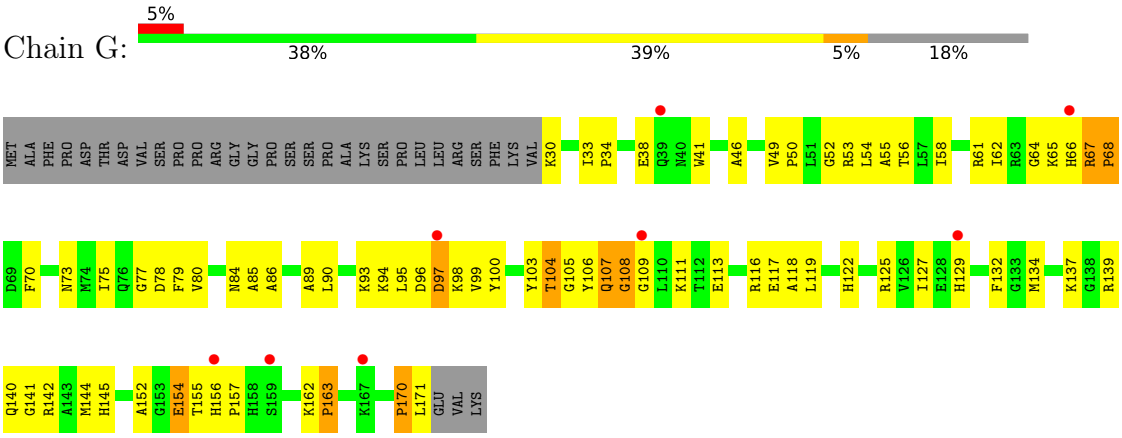
• Molecule 8: 50S ribosomal protein L11

Chain F:



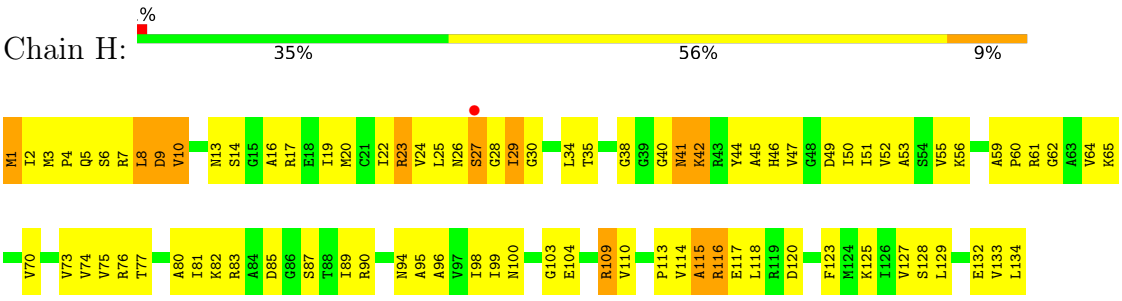
• Molecule 9: 50S ribosomal protein L13

Chain G:



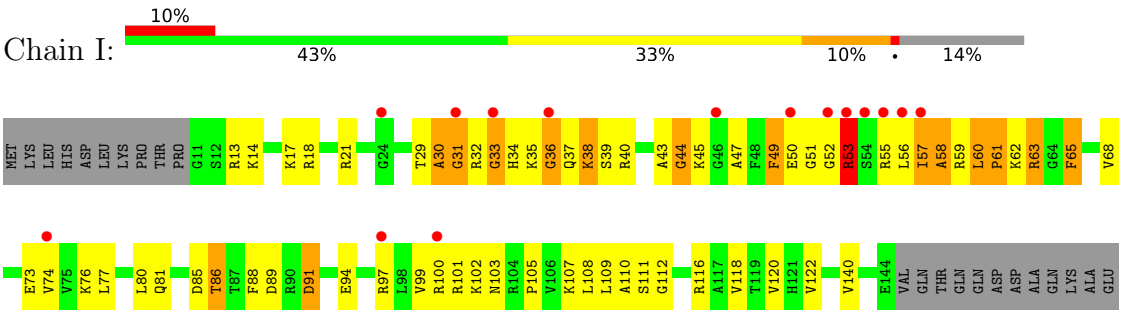
• Molecule 10: 50S ribosomal protein L14

Chain H:



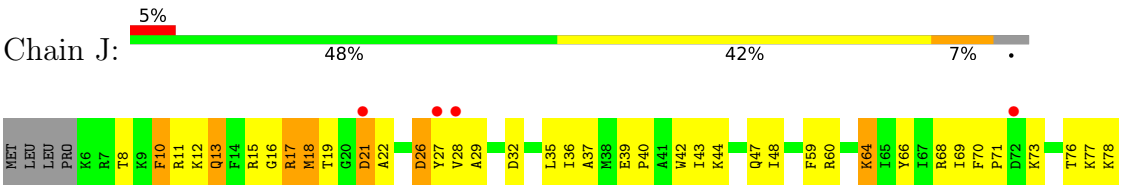
• Molecule 11: 50S ribosomal protein L15

Chain I:



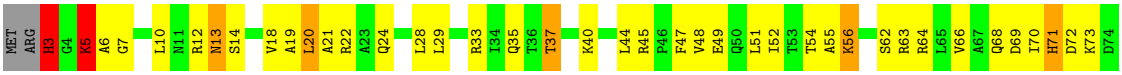
• Molecule 12: 50S ribosomal protein L16

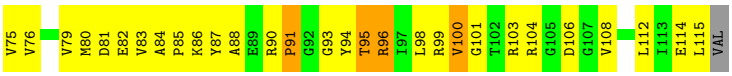
Chain J:



• Molecule 13: 50S ribosomal protein L17

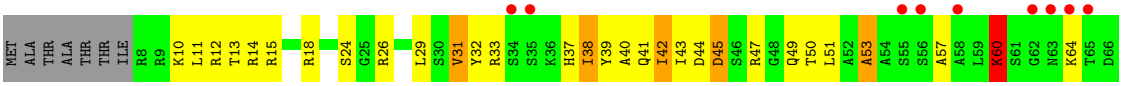
Chain K:

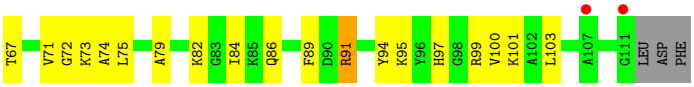




• Molecule 14: 50S ribosomal protein L18

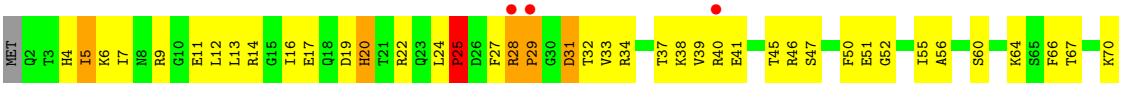
Chain L:





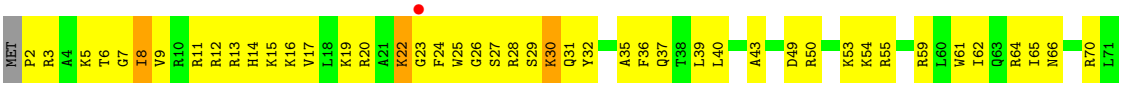
• Molecule 15: 50S ribosomal protein L19

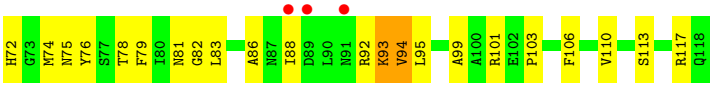
Chain M:



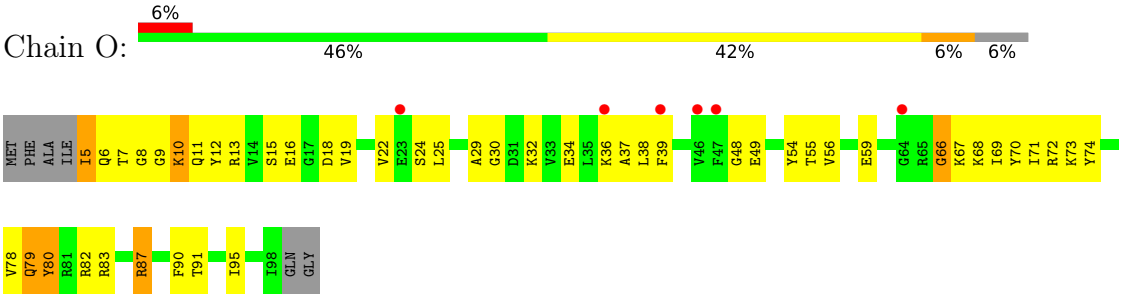
• Molecule 16: 50S ribosomal protein L20

Chain N:

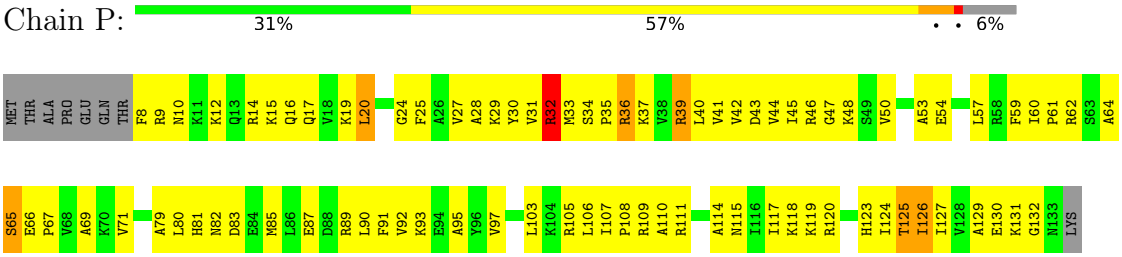




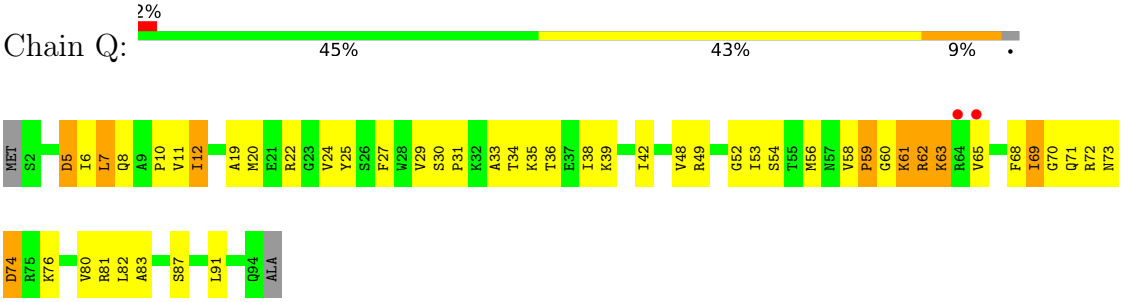
• Molecule 17: 50S ribosomal protein L21



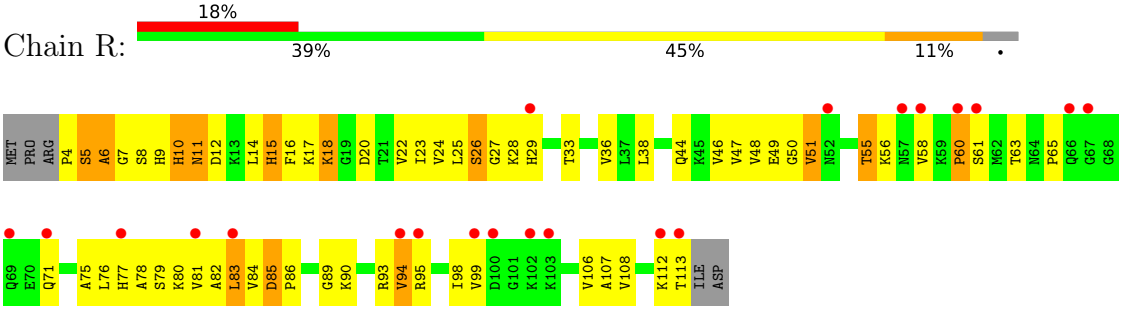
• Molecule 18: 50S ribosomal protein L22



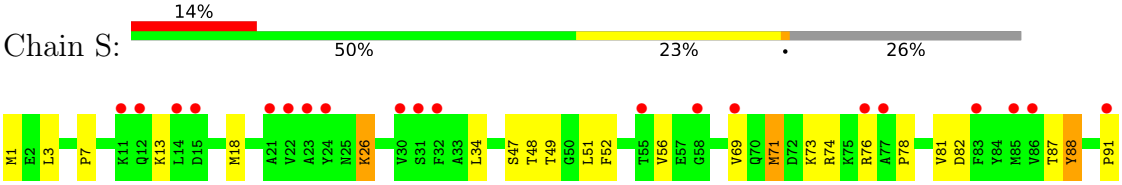
• Molecule 19: 50S ribosomal protein L23

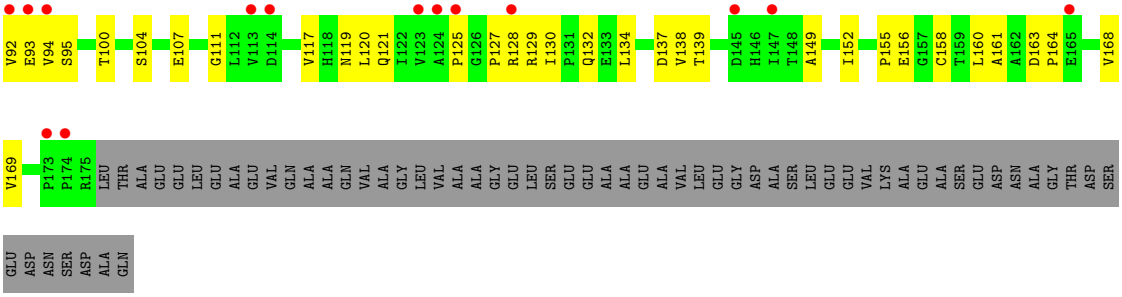


• Molecule 20: 50S ribosomal protein L24

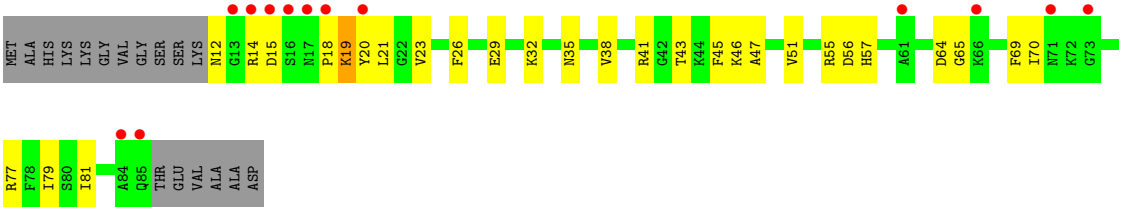


• Molecule 21: 50S ribosomal protein L25

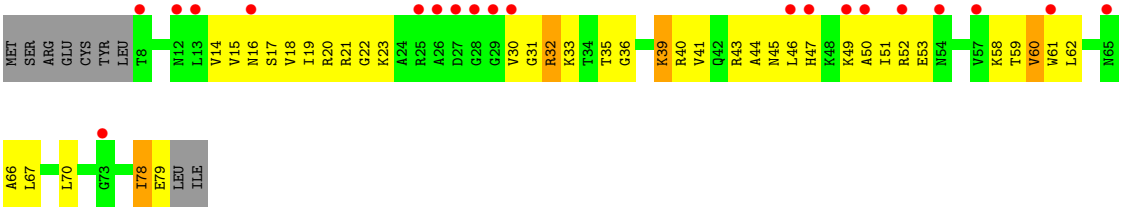




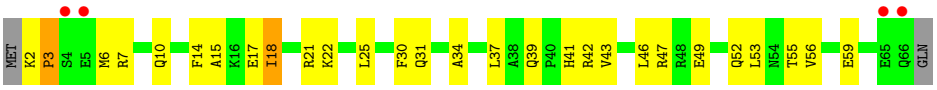
• Molecule 22: 50S ribosomal protein L27



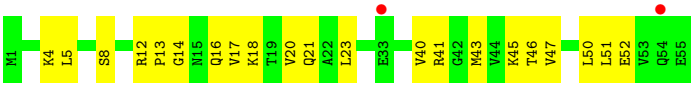
• Molecule 23: 50S ribosomal protein L28



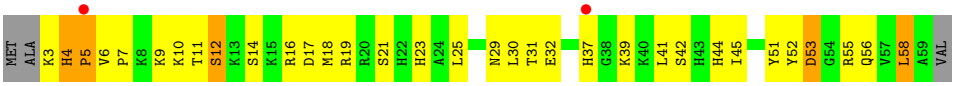
• Molecule 24: 50S ribosomal protein L29



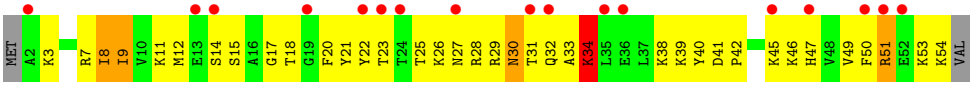
• Molecule 25: 50S ribosomal protein L30



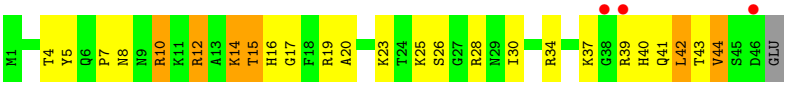
• Molecule 26: 50S ribosomal protein L32



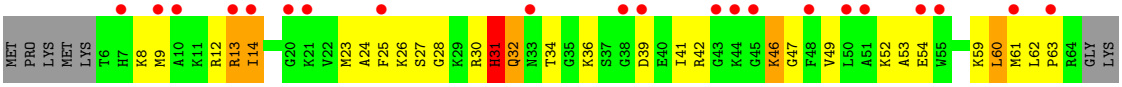
• Molecule 27: 50S ribosomal protein L33



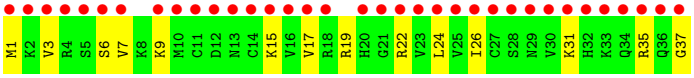
• Molecule 28: 50S ribosomal protein L34



• Molecule 29: 50S ribosomal protein L35



• Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	170.59Å 410.20Å 695.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25 34.75 – 3.25	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-3.25) 93.3 (34.75-3.25)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.252 , 0.294 0.258 , 0.297	Depositor DCC
R_{free} test set	3585 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å^2)	73.8	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 65.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	84383	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: NA, K, MG, LMA

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	0.69	12/63867 (0.0%)	1.28	804/99618 (0.8%)
2	Y	0.46	0/2863	0.86	5/4461 (0.1%)
3	A	0.49	1/1958 (0.1%)	0.65	2/2638 (0.1%)
4	B	0.55	0/1567	0.79	0/2105
5	C	0.52	0/1504	0.67	0/2036
6	D	0.31	0/1419	0.45	0/1903
7	E	0.33	0/1308	0.48	0/1771
8	F	0.22	0/455	0.37	0/611
9	G	0.57	0/1138	0.70	0/1539
10	H	0.63	0/1007	0.84	0/1352
11	I	0.54	0/1022	0.64	0/1366
12	J	0.48	0/1113	0.63	0/1486
13	K	0.81	1/886 (0.1%)	1.06	6/1188 (0.5%)
14	L	0.40	0/785	0.56	0/1048
15	M	0.67	0/884	0.88	1/1186 (0.1%)
16	N	0.55	0/994	0.71	0/1323
17	O	0.44	0/750	0.62	0/1000
18	P	0.58	0/1017	0.79	1/1362 (0.1%)
19	Q	0.47	0/737	0.63	0/988
20	R	0.45	0/835	0.59	0/1121
21	S	0.33	0/1370	0.48	0/1862
22	T	0.43	0/563	0.56	0/747
23	U	0.40	0/556	0.58	0/741
24	V	0.31	0/529	0.47	0/704
25	W	0.39	0/426	0.65	0/568
26	Z	0.56	0/464	0.79	0/622
27	1	0.48	0/438	0.56	0/583
28	2	0.56	0/387	0.71	0/509
29	3	0.59	0/468	0.65	0/614
30	4	0.22	0/298	0.37	0/390
All	All	0.63	14/91608 (0.0%)	1.15	819/137442 (0.6%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1977	C	P-O5'	-7.09	1.52	1.59
1	X	774	A	N7-C5	7.06	1.43	1.39
1	X	1333	G	O3'-P	-6.43	1.53	1.61
1	X	1202	U	O3'-P	-6.42	1.53	1.61
1	X	774	A	N9-C8	6.38	1.42	1.37
1	X	1975	G	C6-N1	-6.25	1.35	1.39
1	X	1688	U	C2-N3	6.11	1.42	1.37
1	X	774	A	N3-C4	6.01	1.38	1.34
1	X	2857	C	N1-C6	-6.01	1.33	1.37
1	X	577	U	C4-O4	5.82	1.28	1.23
13	K	3	HIS	CA-C	5.60	1.67	1.52
1	X	2398	U	C2-N3	-5.53	1.33	1.37
3	A	248	VAL	CB-CG2	-5.21	1.42	1.52
1	X	1467	U	N1-C2	5.12	1.43	1.38

All (819) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1975	G	N1-C6-O6	-19.89	107.97	119.90
1	X	774	A	C5-N7-C8	-17.57	95.12	103.90
1	X	774	A	C4-C5-C6	-17.47	108.26	117.00
1	X	1670	G	C8-N9-C4	15.74	112.69	106.40
1	X	774	A	C4-C5-N7	14.89	118.15	110.70
1	X	1679	U	C5-C6-N1	-14.87	115.27	122.70
1	X	1683	G	N1-C6-O6	-14.47	111.22	119.90
1	X	1467	U	N3-C2-O2	-14.36	112.15	122.20
1	X	2480	C	N3-C2-O2	13.37	131.26	121.90
1	X	1305	C	C6-N1-C2	12.91	125.46	120.30
1	X	1683	G	C5-C6-O6	12.88	136.33	128.60
1	X	774	A	N1-C2-N3	-12.52	123.04	129.30
1	X	1670	G	N7-C8-N9	-12.50	106.85	113.10
1	X	2548	G	N1-C6-O6	-12.12	112.63	119.90
1	X	2480	C	N1-C2-O2	-11.88	111.77	118.90
1	X	774	A	N7-C8-N9	11.32	119.46	113.80
1	X	1266	G	C5-N7-C8	11.31	109.95	104.30
1	X	968	C	N1-C2-O2	11.09	125.56	118.90
1	X	989	G	C8-N9-C4	11.06	110.82	106.40
1	X	1663	C	N1-C2-O2	10.96	125.48	118.90
1	X	1975	G	C5-C6-N1	10.95	116.97	111.50
1	X	2703	C	C6-N1-C2	10.84	124.64	120.30
1	X	2634	G	C8-N9-C4	10.81	110.72	106.40
1	X	1975	G	C5-C6-O6	10.74	135.04	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1266	G	C4-C5-N7	-10.72	106.51	110.80
1	X	1982	C	C5-C6-N1	-10.67	115.67	121.00
1	X	2666	U	C5-C6-N1	-10.63	117.39	122.70
1	X	1674	C	C5-C6-N1	-10.58	115.71	121.00
1	X	1288	A	C5-C6-N1	-10.57	112.42	117.70
1	X	1467	U	N1-C2-O2	10.44	130.11	122.80
1	X	1288	A	C2-N3-C4	-10.44	105.38	110.60
1	X	527	C	N1-C2-O2	10.41	125.14	118.90
1	X	2805	G	N1-C6-O6	-10.28	113.73	119.90
1	X	1674	C	C6-N1-C2	10.24	124.40	120.30
1	X	1291	G	C8-N9-C4	10.18	110.47	106.40
1	X	559	C	C5-C6-N1	10.15	126.07	121.00
1	X	2590	U	C4-C5-C6	10.12	125.77	119.70
1	X	522	G	N1-C6-O6	10.07	125.94	119.90
1	X	2590	U	N1-C2-N3	9.93	120.86	114.90
1	X	577	U	N3-C4-C5	-9.82	108.71	114.60
1	X	2398	U	N3-C4-C5	9.73	120.44	114.60
1	X	774	A	C5-C6-N1	9.68	122.54	117.70
1	X	2590	U	N1-C2-O2	-9.54	116.12	122.80
1	X	1679	U	C2-N3-C4	-9.46	121.33	127.00
1	X	1266	G	N7-C8-N9	-9.40	108.40	113.10
1	X	1212	U	C5-C6-N1	-9.39	118.00	122.70
1	X	2618	A	N1-C2-N3	9.38	133.99	129.30
1	X	1981	A	N7-C8-N9	-9.28	109.16	113.80
1	X	1676	U	C5-C6-N1	-9.23	118.08	122.70
1	X	503	G	C8-N9-C4	9.13	110.05	106.40
1	X	1981	A	C5-N7-C8	9.13	108.46	103.90
1	X	2815	C	C6-N1-C2	9.12	123.95	120.30
1	X	789	G	N1-C6-O6	9.11	125.37	119.90
1	X	1309	G	C8-N9-C4	9.09	110.04	106.40
1	X	1211	G	C8-N9-C4	9.07	110.03	106.40
1	X	2815	C	C5-C6-N1	-9.07	116.46	121.00
1	X	796	A	N1-C6-N6	9.06	124.03	118.60
1	X	538	A	C2-N3-C4	8.99	115.09	110.60
1	X	2846	G	C8-N9-C4	8.97	109.99	106.40
1	X	1770	U	C5-C6-N1	-8.96	118.22	122.70
1	X	2665	G	N7-C8-N9	-8.95	108.63	113.10
1	X	2665	G	C8-N9-C4	8.89	109.96	106.40
1	X	2807	U	C5-C6-N1	-8.88	118.26	122.70
1	X	2553	G	C8-N9-C4	-8.88	102.85	106.40
1	X	774	A	N9-C4-C5	-8.85	102.26	105.80
1	X	2038	C	N1-C2-O2	8.83	124.20	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2548	G	C5-C6-O6	8.76	133.85	128.60
1	X	2705	A	C8-N9-C4	8.76	109.30	105.80
1	X	1702	C	C6-N1-C2	8.73	123.79	120.30
1	X	1660	G	N1-C6-O6	-8.71	114.68	119.90
1	X	559	C	C2-N3-C4	8.65	124.23	119.90
1	X	1743	C	C5-C6-N1	-8.65	116.68	121.00
1	X	1982	C	C4-C5-C6	8.63	121.72	117.40
1	X	1937	G	C8-N9-C4	8.62	109.85	106.40
3	A	248	VAL	CG1-CB-CG2	-8.59	97.16	110.90
1	X	989	G	N7-C8-N9	-8.57	108.82	113.10
1	X	2712	G	N1-C6-O6	-8.56	114.77	119.90
1	X	1279	G	N7-C8-N9	-8.53	108.83	113.10
1	X	1968	G	C8-N9-C4	8.48	109.79	106.40
1	X	2496	C	N3-C4-C5	8.46	125.28	121.90
1	X	1678	G	N1-C6-O6	-8.45	114.83	119.90
1	X	2597	G	C5-C6-O6	8.38	133.63	128.60
1	X	1662	G	N1-C6-O6	-8.37	114.88	119.90
1	X	1670	G	C5-N7-C8	8.30	108.45	104.30
1	X	2689	C	C6-N1-C2	8.23	123.59	120.30
1	X	1688	U	N3-C4-O4	8.14	125.10	119.40
1	X	1993	G	C2-N3-C4	-8.12	107.84	111.90
1	X	2792	C	C5-C6-N1	-8.08	116.96	121.00
1	X	1966	C	C5-C6-N1	-8.07	116.96	121.00
1	X	2033	C	N3-C2-O2	-8.07	116.25	121.90
1	X	1981	A	C8-N9-C4	8.05	109.02	105.80
1	X	1278	A	C8-N9-C4	-8.04	102.59	105.80
1	X	961	G	C5-C6-O6	8.03	133.42	128.60
1	X	1305	C	C5-C6-N1	-8.03	116.99	121.00
1	X	1653	C	C6-N1-C2	8.03	123.51	120.30
1	X	787	A	C2-N3-C4	-8.02	106.59	110.60
1	X	2713	A	C8-N9-C4	8.01	109.00	105.80
1	X	1978	U	N1-C2-O2	-8.01	117.19	122.80
1	X	1279	G	C5-N7-C8	7.99	108.30	104.30
1	X	538	A	C5-C6-N1	7.94	121.67	117.70
1	X	2809	A	C5-C6-N6	-7.94	117.35	123.70
1	X	1700	C	C6-N1-C2	7.92	123.47	120.30
1	X	1291	G	N7-C8-N9	-7.92	109.14	113.10
1	X	2478	C	C6-N1-C2	-7.92	117.13	120.30
1	X	741	G	N7-C8-N9	-7.91	109.15	113.10
1	X	1702	C	C5-C6-N1	-7.86	117.07	121.00
1	X	559	C	C6-N1-C2	-7.83	117.17	120.30
1	X	1680	U	C5-C6-N1	-7.83	118.78	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	689	A	C5-N7-C8	-7.83	99.99	103.90
1	X	2681	A	N1-C6-N6	7.82	123.29	118.60
1	X	741	G	C8-N9-C4	7.80	109.52	106.40
1	X	1984	A	N1-C6-N6	-7.79	113.93	118.60
1	X	2665	G	C5-N7-C8	7.78	108.19	104.30
1	X	1679	U	C6-N1-C2	7.76	125.66	121.00
1	X	1991	C	C5-C6-N1	-7.76	117.12	121.00
1	X	1984	A	N1-C2-N3	7.76	133.18	129.30
1	X	1975	G	C6-N1-C2	-7.69	120.49	125.10
1	X	2703	C	C5-C6-N1	-7.68	117.16	121.00
1	X	2590	U	C5-C6-N1	-7.67	118.86	122.70
1	X	1655	C	C5-C6-N1	-7.67	117.17	121.00
1	X	2855	C	N3-C2-O2	7.67	127.27	121.90
1	X	968	C	C2-N1-C1'	7.63	127.19	118.80
1	X	2655	C	C6-N1-C2	7.63	123.35	120.30
1	X	2247	A	N1-C6-N6	7.61	123.17	118.60
1	X	520	C	N1-C2-O2	-7.58	114.35	118.90
1	X	1642	G	C2-N3-C4	-7.57	108.11	111.90
1	X	1278	A	N7-C8-N9	7.55	117.57	113.80
1	X	1980	A	C5-N7-C8	7.54	107.67	103.90
1	X	1212	U	C5-C4-O4	7.53	130.42	125.90
1	X	2493	U	C5-C6-N1	-7.53	118.93	122.70
1	X	2023	C	C6-N1-C2	7.51	123.31	120.30
1	X	1982	C	C2-N3-C4	-7.50	116.15	119.90
1	X	1211	G	N9-C4-C5	-7.48	102.41	105.40
1	X	2701	A	N1-C2-N3	7.46	133.03	129.30
1	X	1304	U	C5-C6-N1	-7.46	118.97	122.70
1	X	1995	G	C8-N9-C4	7.46	109.38	106.40
1	X	2705	A	N9-C4-C5	-7.45	102.82	105.80
1	X	542	A	N1-C6-N6	7.44	123.07	118.60
1	X	1305	C	N3-C2-O2	7.42	127.09	121.90
1	X	2430	A	N1-C6-N6	-7.41	114.16	118.60
1	X	968	C	C6-N1-C1'	-7.40	111.92	120.80
1	X	1674	C	N3-C4-C5	7.37	124.85	121.90
1	X	1270	C	N3-C4-C5	-7.35	118.96	121.90
1	X	1674	C	C2-N3-C4	-7.34	116.23	119.90
1	X	1700	C	C5-C6-N1	-7.34	117.33	121.00
1	X	1993	G	N1-C6-O6	7.33	124.30	119.90
1	X	825	C	C6-N1-C2	7.32	123.23	120.30
1	X	1674	C	N3-C4-N4	-7.32	112.88	118.00
18	P	32	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	X	1211	G	N3-C2-N2	7.30	125.01	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2805	G	C5-C6-O6	7.28	132.97	128.60
1	X	538	A	N1-C2-N3	-7.28	125.66	129.30
1	X	1683	G	C6-C5-N7	7.27	134.76	130.40
1	X	1275	A	N1-C6-N6	7.27	122.96	118.60
1	X	2766	U	C5-C6-N1	-7.26	119.07	122.70
1	X	1928	G	N1-C6-O6	-7.26	115.55	119.90
1	X	1622	G	N1-C6-O6	-7.25	115.55	119.90
1	X	787	A	C5-C6-N1	-7.25	114.08	117.70
1	X	1748	U	N3-C2-O2	7.24	127.27	122.20
1	X	1142	G	N3-C2-N2	7.23	124.96	119.90
1	X	1467	U	C4-C5-C6	7.22	124.03	119.70
1	X	1743	C	C6-N1-C2	7.22	123.19	120.30
1	X	1775	A	C8-N9-C4	7.22	108.69	105.80
1	X	527	C	C6-N1-C2	-7.21	117.42	120.30
1	X	2748	C	C6-N1-C2	7.20	123.18	120.30
1	X	1989	C	N3-C2-O2	7.17	126.92	121.90
1	X	542	A	N7-C8-N9	7.16	117.38	113.80
1	X	2671	C	C6-N1-C2	-7.14	117.44	120.30
1	X	1937	G	N7-C8-N9	-7.14	109.53	113.10
1	X	2717	G	C5-C6-N1	7.13	115.07	111.50
1	X	966	A	N1-C6-N6	7.13	122.88	118.60
1	X	1341	G	C8-N9-C4	7.12	109.25	106.40
1	X	2398	U	N3-C4-O4	-7.12	114.42	119.40
1	X	1278	A	N1-C6-N6	7.10	122.86	118.60
1	X	2611	A	C8-N9-C4	7.10	108.64	105.80
1	X	961	G	N1-C6-O6	-7.10	115.64	119.90
1	X	2040	A	C8-N9-C4	7.10	108.64	105.80
1	X	825	C	N1-C2-O2	-7.10	114.64	118.90
1	X	1305	C	N1-C2-O2	-7.08	114.65	118.90
1	X	2809	A	C5-C6-N1	7.06	121.23	117.70
1	X	1279	G	C8-N9-C4	7.06	109.22	106.40
1	X	2820	C	N3-C4-N4	-7.06	113.06	118.00
1	X	1245	G	N1-C6-O6	-7.05	115.67	119.90
1	X	545	C	C5-C6-N1	-7.04	117.48	121.00
1	X	2423	G	N1-C6-O6	-7.03	115.68	119.90
1	X	2765	C	C5-C6-N1	-7.03	117.48	121.00
1	X	1972	G	C8-N9-C4	-7.03	103.59	106.40
1	X	1289	A	N9-C4-C5	-7.02	102.99	105.80
1	X	1471	G	C5-C6-N1	7.01	115.01	111.50
1	X	2569	A	C8-N9-C4	7.01	108.60	105.80
1	X	1321	A	C8-N9-C4	7.01	108.60	105.80
1	X	883	A	C8-N9-C4	7.00	108.60	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1286	U	N1-C2-O2	-7.00	117.90	122.80
1	X	1679	U	C4-C5-C6	7.00	123.90	119.70
1	X	1663	C	N1-C2-N3	-6.99	114.31	119.20
1	X	789	G	C5-C6-O6	-6.99	124.41	128.60
1	X	799	C	C6-N1-C2	6.98	123.09	120.30
1	X	1989	C	C4-C5-C6	-6.97	113.91	117.40
1	X	2702	G	N1-C6-O6	-6.96	115.72	119.90
1	X	2551	A	C8-N9-C4	6.95	108.58	105.80
13	K	99	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	X	2741	G	C8-N9-C4	6.92	109.17	106.40
1	X	2793	G	C8-N9-C4	6.91	109.16	106.40
1	X	527	C	N3-C2-O2	-6.91	117.06	121.90
1	X	1720	G	C8-N9-C4	6.91	109.16	106.40
1	X	1766	U	C5-C6-N1	-6.90	119.25	122.70
1	X	2600	A	N1-C6-N6	-6.90	114.46	118.60
1	X	2520	A	N1-C6-N6	-6.89	114.47	118.60
1	X	741	G	C5-N7-C8	6.88	107.74	104.30
1	X	2634	G	N7-C8-N9	-6.88	109.66	113.10
1	X	746	G	N1-C6-O6	-6.87	115.78	119.90
1	X	757	U	C5-C6-N1	-6.87	119.26	122.70
1	X	2807	U	C6-N1-C2	6.87	125.12	121.00
1	X	840	U	C5-C6-N1	-6.87	119.27	122.70
1	X	1633	C	C6-N1-C2	6.87	123.05	120.30
1	X	802	A	N1-C6-N6	6.86	122.72	118.60
1	X	1682	A	C2-N3-C4	6.86	114.03	110.60
1	X	542	A	C5-N7-C8	-6.86	100.47	103.90
1	X	1324	G	N1-C6-O6	6.85	124.01	119.90
1	X	545	C	C6-N1-C2	6.85	123.04	120.30
1	X	1670	G	N3-C4-C5	6.85	132.02	128.60
1	X	2559	U	N3-C4-O4	6.84	124.19	119.40
1	X	1773	C	N1-C2-O2	6.83	123.00	118.90
1	X	1471	G	N3-C4-N9	6.83	130.10	126.00
1	X	841	G	C4-C5-N7	6.82	113.53	110.80
1	X	841	G	C5-N7-C8	-6.79	100.90	104.30
1	X	1676	U	C6-N1-C2	6.77	125.06	121.00
1	X	1920	A	C8-N9-C4	6.76	108.50	105.80
1	X	1655	C	C6-N1-C2	6.76	123.00	120.30
1	X	2655	C	C5-C6-N1	-6.75	117.63	121.00
1	X	527	C	C5-C6-N1	6.73	124.36	121.00
1	X	2467	A	N1-C6-N6	-6.73	114.56	118.60
1	X	1920	A	N7-C8-N9	-6.73	110.44	113.80
1	X	2852	G	C8-N9-C4	6.71	109.08	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1966	C	C6-N1-C2	6.70	122.98	120.30
1	X	1968	G	N7-C8-N9	-6.70	109.75	113.10
1	X	577	U	C4-C5-C6	6.69	123.72	119.70
1	X	1576	G	C8-N9-C4	-6.69	103.72	106.40
1	X	1285	A	C5-C6-N1	-6.68	114.36	117.70
1	X	1339	U	N3-C2-O2	-6.67	117.53	122.20
1	X	559	C	N3-C4-C5	-6.66	119.24	121.90
1	X	1748	U	C6-N1-C2	6.66	124.99	121.00
1	X	544	U	N3-C2-O2	-6.65	117.54	122.20
1	X	1931	G	C8-N9-C4	-6.63	103.75	106.40
1	X	2007	G	C4-C5-N7	-6.63	108.15	110.80
1	X	2495	G	N1-C6-O6	-6.62	115.93	119.90
1	X	2398	U	C2-N3-C4	-6.61	123.03	127.00
1	X	1653	C	C5-C6-N1	-6.61	117.70	121.00
1	X	477	A	C8-N9-C4	6.60	108.44	105.80
1	X	1988	A	C8-N9-C4	6.60	108.44	105.80
1	X	196	A	N1-C6-N6	-6.60	114.64	118.60
1	X	1770	U	C5-C4-O4	6.60	129.86	125.90
1	X	951	G	N1-C6-O6	-6.59	115.95	119.90
1	X	936	A	N1-C6-N6	-6.59	114.65	118.60
1	X	1975	G	N1-C2-N2	-6.57	110.28	116.20
1	X	841	G	N3-C4-C5	6.57	131.88	128.60
1	X	2418	A	C8-N9-C4	-6.57	103.17	105.80
1	X	699	G	N3-C4-C5	6.57	131.88	128.60
1	X	1822	C	C5-C6-N1	-6.56	117.72	121.00
1	X	465	C	C5-C6-N1	-6.56	117.72	121.00
1	X	825	C	N3-C2-O2	6.56	126.49	121.90
1	X	747	A	C8-N9-C4	6.55	108.42	105.80
1	X	2815	C	N3-C4-N4	-6.55	113.42	118.00
1	X	2623	A	C8-N9-C4	6.54	108.42	105.80
1	X	1309	G	N7-C8-N9	-6.54	109.83	113.10
1	X	1682	A	C5-C6-N6	-6.53	118.48	123.70
1	X	2406	C	N1-C2-O2	-6.51	114.99	118.90
1	X	2792	C	C2-N3-C4	-6.50	116.65	119.90
1	X	1259	A	C8-N9-C4	6.50	108.40	105.80
1	X	1991	C	C4-C5-C6	6.48	120.64	117.40
1	X	695	G	C8-N9-C4	6.48	108.99	106.40
1	X	460	U	C5-C6-N1	6.47	125.94	122.70
1	X	1006	C	N1-C2-O2	6.47	122.78	118.90
1	X	2686	C	C4-C5-C6	6.47	120.63	117.40
1	X	340	G	C8-N9-C4	6.47	108.99	106.40
1	X	1270	C	C4-C5-C6	6.46	120.63	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	550	C	C5-C6-N1	-6.45	117.77	121.00
1	X	2559	U	C5-C4-O4	-6.45	122.03	125.90
1	X	2431	C	N1-C2-O2	6.45	122.77	118.90
1	X	520	C	C6-N1-C2	-6.45	117.72	120.30
1	X	513	A	N1-C2-N3	6.44	132.52	129.30
1	X	2701	A	C2-N3-C4	-6.44	107.38	110.60
1	X	586	G	C8-N9-C4	6.44	108.97	106.40
1	X	581	A	N1-C6-N6	6.41	122.45	118.60
1	X	832	A	N9-C4-C5	-6.40	103.24	105.80
1	X	2760	G	C8-N9-C4	6.39	108.96	106.40
1	X	1571	G	C8-N9-C4	-6.39	103.84	106.40
1	X	691	C	C6-N1-C2	6.39	122.86	120.30
1	X	853	C	C6-N1-C2	6.38	122.85	120.30
1	X	1816	G	C8-N9-C4	6.38	108.95	106.40
1	X	2711	G	C8-N9-C4	6.38	108.95	106.40
1	X	2666	U	C2-N3-C4	-6.37	123.18	127.00
1	X	806	A	N1-C6-N6	-6.37	114.78	118.60
1	X	575	U	C5-C4-O4	6.37	129.72	125.90
1	X	1324	G	C5-C6-O6	-6.36	124.79	128.60
1	X	2718	A	C5-C6-N1	6.35	120.88	117.70
1	X	2704	U	C5-C6-N1	-6.35	119.53	122.70
1	X	2492	G	N3-C4-C5	-6.34	125.43	128.60
1	X	2331	A	N1-C6-N6	-6.34	114.80	118.60
1	X	1816	G	N7-C8-N9	-6.33	109.93	113.10
1	X	1623	C	N1-C2-O2	6.33	122.70	118.90
1	X	2854	G	N1-C6-O6	6.33	123.69	119.90
1	X	1205	G	C8-N9-C4	6.32	108.93	106.40
1	X	1699	A	C2-N3-C4	-6.32	107.44	110.60
1	X	1035	G	C8-N9-C4	-6.31	103.87	106.40
1	X	822	G	N3-C4-C5	-6.31	125.44	128.60
1	X	527	C	C2-N3-C4	6.31	123.05	119.90
1	X	528	G	N1-C6-O6	-6.30	116.12	119.90
1	X	2495	G	N3-C2-N2	6.30	124.31	119.90
1	X	2314	A	C5-C6-N1	6.29	120.85	117.70
1	X	2634	G	N9-C4-C5	-6.29	102.88	105.40
1	X	1974	U	N1-C2-O2	6.29	127.20	122.80
1	X	2553	G	N7-C8-N9	6.28	116.24	113.10
1	X	542	A	C2-N3-C4	-6.28	107.46	110.60
1	X	1540	C	C6-N1-C2	-6.28	117.79	120.30
1	X	1292	A	N1-C2-N3	6.28	132.44	129.30
1	X	1289	A	N1-C6-N6	6.27	122.36	118.60
1	X	2240	C	N3-C2-O2	-6.27	117.51	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1975	G	C8-N9-C1'	-6.26	118.86	127.00
1	X	2846	G	N7-C8-N9	-6.26	109.97	113.10
1	X	1980	A	N1-C6-N6	-6.26	114.84	118.60
1	X	590	C	N3-C4-N4	-6.24	113.63	118.00
1	X	1274	C	C6-N1-C2	6.24	122.80	120.30
1	X	1277	G	C8-N9-C4	6.24	108.90	106.40
1	X	122	G	C2-N3-C4	-6.24	108.78	111.90
1	X	689	A	C4-C5-N7	6.24	113.82	110.70
1	X	1312	G	N1-C6-O6	6.24	123.64	119.90
1	X	808	C	C6-N1-C2	6.23	122.79	120.30
1	X	1981	A	C4-C5-N7	-6.23	107.58	110.70
1	X	537	C	C5-C6-N1	-6.23	117.89	121.00
1	X	2033	C	N1-C2-O2	6.23	122.64	118.90
1	X	2711	G	N7-C8-N9	-6.23	109.99	113.10
1	X	754	G	C8-N9-C4	6.22	108.89	106.40
1	X	2686	C	N3-C2-O2	-6.22	117.54	121.90
1	X	542	A	C8-N9-C4	-6.22	103.31	105.80
1	X	608	G	N7-C8-N9	-6.22	109.99	113.10
1	X	774	A	N3-C4-C5	6.21	131.15	126.80
1	X	774	A	C2-N3-C4	6.21	113.70	110.60
1	X	1996	A	N7-C8-N9	6.19	116.90	113.80
1	X	1682	A	N3-C4-C5	-6.19	122.47	126.80
1	X	1292	A	C8-N9-C4	6.18	108.27	105.80
1	X	1713	G	N1-C6-O6	-6.17	116.19	119.90
1	X	1288	A	C4-C5-C6	6.16	120.08	117.00
1	X	1285	A	C2-N3-C4	-6.15	107.52	110.60
1	X	1291	G	C6-N1-C2	-6.15	121.41	125.10
1	X	1223	G	C2-N3-C4	-6.14	108.83	111.90
1	X	689	A	N7-C8-N9	6.13	116.87	113.80
1	X	2038	C	N3-C2-O2	-6.11	117.62	121.90
1	X	1378	A	C8-N9-C4	6.11	108.24	105.80
1	X	1993	G	C5-C6-N1	-6.11	108.45	111.50
1	X	771	C	N3-C2-O2	-6.10	117.63	121.90
1	X	1288	A	N1-C2-N3	6.10	132.35	129.30
1	X	1622	G	C8-N9-C4	6.09	108.84	106.40
1	X	534	U	C5-C6-N1	-6.09	119.66	122.70
1	X	799	C	C5-C6-N1	-6.09	117.96	121.00
1	X	1266	G	C4-C5-C6	6.08	122.45	118.80
1	X	2314	A	C2-N3-C4	6.08	113.64	110.60
1	X	1663	C	C2-N3-C4	6.08	122.94	119.90
1	X	822	G	C4-C5-N7	-6.07	108.37	110.80
1	X	1622	G	C5-C6-O6	6.07	132.24	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2227	C	N1-C2-O2	-6.07	115.26	118.90
1	X	1278	A	C6-C5-N7	-6.07	128.05	132.30
1	X	1687	C	C4-C5-C6	6.07	120.43	117.40
1	X	1467	U	C5-C6-N1	-6.06	119.67	122.70
1	X	600	G	N1-C6-O6	6.06	123.54	119.90
1	X	808	C	C5-C6-N1	-6.06	117.97	121.00
1	X	522	G	C4-C5-N7	6.06	113.22	110.80
1	X	608	G	C5-N7-C8	6.06	107.33	104.30
1	X	2551	A	N7-C8-N9	-6.06	110.77	113.80
1	X	2597	G	N1-C6-O6	-6.06	116.27	119.90
1	X	522	G	C5-C6-O6	-6.06	124.97	128.60
1	X	2677	U	C5-C6-N1	-6.05	119.67	122.70
1	X	1694	A	C8-N9-C4	6.05	108.22	105.80
1	X	1260	A	C8-N9-C4	6.05	108.22	105.80
1	X	1212	U	N3-C4-O4	-6.04	115.17	119.40
1	X	1015	U	C6-N1-C2	-6.04	117.38	121.00
1	X	497	C	N1-C2-O2	-6.03	115.28	118.90
1	X	1471	G	C5-C6-O6	-6.03	124.98	128.60
1	X	2626	U	N3-C2-O2	-6.02	117.99	122.20
1	X	1676	U	C2-N3-C4	-6.02	123.39	127.00
1	X	1678	G	N7-C8-N9	-6.02	110.09	113.10
1	X	1672	A	N1-C6-N6	6.01	122.21	118.60
1	X	2707	G	N1-C2-N2	6.01	121.61	116.20
1	X	1960	A	C8-N9-C4	6.01	108.20	105.80
1	X	577	U	C2-N3-C4	6.00	130.60	127.00
1	X	957	G	N1-C6-O6	-6.00	116.30	119.90
1	X	832	A	N1-C6-N6	5.99	122.19	118.60
1	X	2629	U	C5-C6-N1	-5.99	119.71	122.70
1	X	155	G	C8-N9-C4	-5.99	104.01	106.40
1	X	974	U	C5-C6-N1	-5.98	119.71	122.70
1	X	966	A	N9-C4-C5	-5.98	103.41	105.80
1	X	713	G	N7-C8-N9	-5.98	110.11	113.10
1	X	1956	G	C8-N9-C4	5.98	108.79	106.40
1	X	2495	G	N3-C4-C5	-5.97	125.61	128.60
1	X	2001	G	C2-N3-C4	-5.97	108.92	111.90
1	X	2688	G	C8-N9-C4	5.96	108.78	106.40
1	X	2854	G	C4-C5-N7	5.96	113.18	110.80
1	X	1652	G	C2-N3-C4	-5.96	108.92	111.90
1	X	552	C	C6-N1-C2	5.96	122.68	120.30
1	X	540	G	C6-N1-C2	5.95	128.67	125.10
1	X	2666	U	C4-C5-C6	5.95	123.27	119.70
1	X	2852	G	C2-N3-C4	-5.95	108.93	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1917	C	N1-C2-O2	5.94	122.46	118.90
1	X	608	G	C8-N9-C4	5.92	108.77	106.40
1	X	1969	G	C5-C6-O6	-5.92	125.05	128.60
1	X	430	C	C6-N1-C2	-5.91	117.94	120.30
1	X	1216	G	N1-C6-O6	-5.91	116.35	119.90
1	X	713	G	C8-N9-C4	5.91	108.76	106.40
1	X	479	G	C8-N9-C4	5.91	108.76	106.40
1	X	1767	G	N1-C6-O6	5.90	123.44	119.90
1	X	1278	A	C5-N7-C8	-5.90	100.95	103.90
1	X	1981	A	C6-N1-C2	-5.90	115.06	118.60
1	X	2822	U	N3-C2-O2	5.90	126.33	122.20
1	X	2258	G	C8-N9-C4	5.90	108.76	106.40
1	X	1699	A	C5-C6-N1	-5.89	114.75	117.70
1	X	1306	U	C2-N3-C4	-5.89	123.47	127.00
1	X	2712	G	C5-C6-O6	5.89	132.13	128.60
1	X	522	G	N3-C4-C5	5.88	131.54	128.60
1	X	544	U	C5-C6-N1	-5.88	119.76	122.70
1	X	1569	A	C6-N1-C2	-5.88	115.07	118.60
1	X	1770	U	N3-C4-O4	-5.88	115.29	119.40
1	X	2791	C	C5-C6-N1	-5.88	118.06	121.00
1	X	1211	G	N1-C2-N2	-5.87	110.92	116.20
1	X	2822	U	C5-C4-O4	-5.87	122.38	125.90
13	K	96	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	X	766	A	N1-C6-N6	-5.86	115.08	118.60
1	X	1680	U	C6-N1-C2	5.86	124.51	121.00
1	X	854	G	N1-C6-O6	5.86	123.41	119.90
1	X	465	C	C4-C5-C6	5.85	120.33	117.40
1	X	716	U	C5-C6-N1	-5.85	119.78	122.70
1	X	883	A	N7-C8-N9	-5.84	110.88	113.80
1	X	2656	G	C8-N9-C4	5.84	108.74	106.40
1	X	1225	G	N1-C6-O6	-5.84	116.40	119.90
1	X	2791	C	C2-N3-C4	-5.84	116.98	119.90
1	X	1272	G	C8-N9-C4	5.84	108.73	106.40
1	X	590	C	C5-C4-N4	5.84	124.28	120.20
1	X	1468	A	N7-C8-N9	-5.83	110.89	113.80
1	X	1678	G	C5-C6-N1	5.82	114.41	111.50
1	X	2370	G	C8-N9-C4	5.82	108.73	106.40
1	X	2710	C	C4-C5-C6	5.82	120.31	117.40
1	X	1578	U	C5-C6-N1	-5.82	119.79	122.70
1	X	1678	G	C5-N7-C8	5.82	107.21	104.30
1	X	748	A	C8-N9-C4	5.81	108.12	105.80
1	X	122	G	N3-C4-C5	5.81	131.50	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	497	C	N3-C2-O2	5.80	125.96	121.90
1	X	2792	C	C4-C5-C6	5.79	120.30	117.40
1	X	1766	U	C6-N1-C2	5.79	124.48	121.00
1	X	2853	U	N3-C4-O4	-5.79	115.34	119.40
1	X	1689	U	C5-C6-N1	-5.78	119.81	122.70
1	X	1974	U	N3-C2-O2	-5.78	118.15	122.20
1	X	1317	G	N1-C6-O6	5.78	123.37	119.90
1	X	1004	A	C8-N9-C4	-5.77	103.49	105.80
1	X	2686	C	C5-C6-N1	-5.76	118.12	121.00
1	X	1998	A	N1-C6-N6	-5.76	115.14	118.60
1	X	1991	C	C5-C4-N4	5.76	124.23	120.20
1	X	1683	G	C4-C5-C6	-5.76	115.35	118.80
1	X	2484	G	C8-N9-C4	-5.76	104.10	106.40
1	X	1996	A	C8-N9-C4	-5.75	103.50	105.80
1	X	609	U	C5-C6-N1	-5.75	119.83	122.70
1	X	1816	G	C5-N7-C8	5.75	107.17	104.30
1	X	2828	C	C5-C4-N4	-5.75	116.18	120.20
13	K	3	HIS	N-CA-C	5.75	126.52	111.00
1	X	814	G	C5-C6-O6	-5.74	125.16	128.60
1	X	789	G	C4-C5-N7	5.74	113.09	110.80
1	X	540	G	N3-C4-C5	5.74	131.47	128.60
1	X	2791	C	C6-N1-C2	5.74	122.59	120.30
1	X	2480	C	C6-N1-C2	5.73	122.59	120.30
1	X	2856	U	C5-C6-N1	5.73	125.57	122.70
1	X	2306	A	N1-C6-N6	5.73	122.04	118.60
1	X	1989	C	N1-C2-O2	-5.72	115.47	118.90
1	X	2703	C	C2-N1-C1'	-5.72	112.51	118.80
1	X	609	U	C6-N1-C2	5.71	124.43	121.00
1	X	2003	A	N1-C6-N6	-5.71	115.18	118.60
1	X	1315	A	N1-C6-N6	-5.70	115.18	118.60
1	X	2637	C	C6-N1-C2	5.70	122.58	120.30
1	X	661	C	C6-N1-C2	-5.70	118.02	120.30
1	X	1291	G	N1-C2-N3	5.70	127.32	123.90
1	X	2495	G	C5-C6-N1	5.70	114.35	111.50
1	X	2655	C	C2-N3-C4	-5.70	117.05	119.90
1	X	974	U	C4-C5-C6	5.70	123.12	119.70
1	X	1270	C	C6-N1-C2	-5.70	118.02	120.30
1	X	2590	U	N3-C4-C5	-5.70	111.18	114.60
1	X	579	G	C4-C5-N7	-5.69	108.52	110.80
1	X	57	G	C8-N9-C4	-5.69	104.12	106.40
1	X	490	A	C5-C6-N1	5.69	120.55	117.70
1	X	1669	A	C8-N9-C4	5.69	108.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2700	U	C5-C6-N1	-5.69	119.86	122.70
1	X	1642	G	C5-C6-N1	-5.69	108.66	111.50
1	X	1290	A	C8-N9-C4	5.68	108.07	105.80
1	X	1622	G	N7-C8-N9	-5.67	110.26	113.10
1	X	1277	G	N3-C2-N2	5.67	123.87	119.90
1	X	2371	A	C8-N9-C4	-5.67	103.53	105.80
1	X	1625	A	C2-N3-C4	-5.67	107.77	110.60
1	X	2430	A	C5-C6-N6	5.67	128.23	123.70
1	X	985	G	N3-C4-C5	-5.66	125.77	128.60
1	X	590	C	N3-C2-O2	-5.66	117.94	121.90
1	X	2710	C	C5-C6-N1	-5.66	118.17	121.00
1	X	691	C	C5-C6-N1	-5.66	118.17	121.00
1	X	1288	A	N1-C6-N6	5.66	122.00	118.60
1	X	1682	A	C6-N1-C2	-5.66	115.20	118.60
1	X	2403	C	C4-C5-C6	5.66	120.23	117.40
1	X	1006	C	N3-C2-O2	-5.66	117.94	121.90
1	X	502	A	C8-N9-C4	5.65	108.06	105.80
1	X	1344	C	N3-C4-C5	5.65	124.16	121.90
1	X	2681	A	C5-C6-N6	-5.65	119.18	123.70
1	X	2592	U	C5-C6-N1	-5.64	119.88	122.70
1	X	229	G	N3-C4-C5	5.64	131.42	128.60
1	X	2756	A	C6-N1-C2	-5.64	115.22	118.60
1	X	1932	G	C4-C5-N7	-5.63	108.55	110.80
1	X	1344	C	N1-C2-O2	5.63	122.28	118.90
1	X	1665	C	N3-C4-N4	-5.63	114.06	118.00
1	X	2060	A	C2-N3-C4	5.62	113.41	110.60
1	X	1750	A	C6-N1-C2	-5.62	115.23	118.60
1	X	2223	U	C5-C6-N1	-5.62	119.89	122.70
1	X	2705	A	N1-C6-N6	5.61	121.97	118.60
1	X	1664	G	N3-C4-C5	5.60	131.40	128.60
1	X	1988	A	N7-C8-N9	-5.60	111.00	113.80
2	Y	92	G	C8-N9-C4	5.60	108.64	106.40
1	X	472	C	N1-C2-O2	-5.60	115.54	118.90
1	X	2739	G	C2-N3-C4	5.60	114.70	111.90
1	X	1256	C	C5-C6-N1	-5.60	118.20	121.00
1	X	2681	A	C4-C5-N7	5.60	113.50	110.70
1	X	2669	C	N3-C4-C5	-5.60	119.66	121.90
1	X	556	A	N1-C6-N6	5.59	121.96	118.60
1	X	1991	C	N3-C4-N4	-5.59	114.08	118.00
1	X	985	G	C8-N9-C4	-5.59	104.16	106.40
1	X	1289	A	C8-N9-C4	5.58	108.03	105.80
1	X	1745	C	N1-C2-O2	-5.58	115.55	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1672	A	C5-C6-N6	-5.58	119.24	123.70
1	X	2549	G	N7-C8-N9	-5.58	110.31	113.10
1	X	2003	A	C2-N3-C4	5.58	113.39	110.60
1	X	822	G	C5-N7-C8	5.57	107.09	104.30
1	X	503	G	N7-C8-N9	-5.57	110.31	113.10
1	X	674	U	N1-C2-O2	-5.57	118.90	122.80
1	X	2713	A	N7-C8-N9	-5.57	111.02	113.80
1	X	1688	U	N3-C4-C5	-5.56	111.26	114.60
1	X	577	U	C5-C4-O4	5.56	129.24	125.90
1	X	961	G	C4-C5-N7	-5.56	108.58	110.80
1	X	236	C	C6-N1-C2	-5.55	118.08	120.30
1	X	39	C	C6-N1-C2	-5.55	118.08	120.30
1	X	1573	G	N1-C6-O6	-5.55	116.57	119.90
1	X	766	A	C6-N1-C2	-5.55	115.27	118.60
1	X	1292	A	C2-N3-C4	-5.55	107.83	110.60
1	X	1625	A	C5-C6-N1	-5.54	114.93	117.70
1	X	1204	G	N3-C4-C5	-5.54	125.83	128.60
1	X	550	C	C2-N3-C4	-5.54	117.13	119.90
1	X	2671	C	C5-C6-N1	5.54	123.77	121.00
1	X	827	C	C6-N1-C2	5.54	122.52	120.30
1	X	1769	U	C5-C6-N1	-5.53	119.93	122.70
1	X	1142	G	N9-C4-C5	-5.53	103.19	105.40
1	X	1670	G	N9-C4-C5	-5.53	103.19	105.40
1	X	2753	C	N1-C2-O2	-5.53	115.58	118.90
1	X	460	U	C6-N1-C2	-5.53	117.68	121.00
1	X	1685	A	C5-C6-N1	5.53	120.46	117.70
1	X	343	A	C8-N9-C4	-5.52	103.59	105.80
1	X	809	C	C5-C6-N1	-5.52	118.24	121.00
1	X	2342	U	C5-C6-N1	-5.52	119.94	122.70
1	X	804	C	C5-C6-N1	-5.51	118.24	121.00
1	X	1341	G	N9-C4-C5	-5.51	103.19	105.40
1	X	1265	G	C5-N7-C8	5.51	107.06	104.30
1	X	1468	A	N1-C6-N6	-5.51	115.29	118.60
1	X	802	A	C2-N3-C4	-5.51	107.84	110.60
1	X	608	G	C4-C5-N7	-5.51	108.60	110.80
1	X	1412	C	N3-C2-O2	5.51	125.75	121.90
1	X	2475	C	C6-N1-C2	-5.51	118.10	120.30
1	X	2765	C	N3-C4-N4	-5.51	114.14	118.00
1	X	1980	A	N7-C8-N9	-5.50	111.05	113.80
1	X	577	U	C6-N1-C2	-5.49	117.70	121.00
13	K	99	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	X	165	G	C8-N9-C4	5.49	108.60	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2707	G	N1-C6-O6	5.49	123.19	119.90
1	X	37	C	C6-N1-C2	-5.49	118.11	120.30
1	X	1176	U	C5-C6-N1	-5.49	119.96	122.70
1	X	1633	C	C5-C6-N1	-5.49	118.26	121.00
1	X	2716	G	C4-C5-N7	-5.48	108.61	110.80
1	X	2432	A	N7-C8-N9	5.48	116.54	113.80
1	X	2854	G	C5-C6-O6	-5.48	125.31	128.60
1	X	814	G	N1-C6-O6	5.47	123.18	119.90
1	X	2240	C	N1-C2-O2	5.47	122.18	118.90
1	X	2685	A	C2-N3-C4	-5.47	107.87	110.60
1	X	2686	C	C2-N3-C4	-5.47	117.17	119.90
1	X	2486	C	C6-N1-C2	-5.46	118.11	120.30
1	X	1025	A	N1-C6-N6	-5.46	115.32	118.60
2	Y	83	C	N3-C4-C5	-5.46	119.72	121.90
1	X	1999	U	C6-N1-C2	5.46	124.28	121.00
1	X	741	G	C4-C5-N7	-5.46	108.62	110.80
1	X	1977	C	N3-C4-N4	5.46	121.82	118.00
1	X	1966	C	C2-N3-C4	-5.46	117.17	119.90
1	X	1226	A	C2-N3-C4	-5.45	107.88	110.60
1	X	2496	C	C6-N1-C2	5.44	122.48	120.30
1	X	1472	C	C6-N1-C2	5.43	122.47	120.30
1	X	559	C	N3-C4-N4	5.43	121.80	118.00
1	X	2793	G	N7-C8-N9	-5.43	110.39	113.10
1	X	229	G	C8-N9-C4	5.43	108.57	106.40
1	X	2663	U	C5-C4-O4	5.43	129.16	125.90
1	X	1293	A	C8-N9-C4	5.41	107.97	105.80
1	X	2787	A	N1-C2-N3	5.41	132.01	129.30
1	X	789	G	C6-C5-N7	-5.41	127.15	130.40
1	X	2331	A	C5-C6-N6	5.41	128.03	123.70
1	X	2852	G	N1-C2-N3	5.41	127.15	123.90
1	X	2851	G	C8-N9-C4	5.41	108.56	106.40
1	X	1975	G	N3-C4-N9	5.40	129.24	126.00
1	X	699	G	C5-N7-C8	-5.40	101.60	104.30
1	X	1260	A	N1-C6-N6	-5.40	115.36	118.60
1	X	1344	C	C6-N1-C2	5.39	122.46	120.30
1	X	1995	G	N7-C8-N9	-5.39	110.40	113.10
1	X	989	G	C5-N7-C8	5.39	107.00	104.30
1	X	471	A	C8-N9-C4	5.39	107.95	105.80
1	X	2716	G	C5-N7-C8	5.39	106.99	104.30
1	X	788	G	C5-C6-N1	5.38	114.19	111.50
1	X	406	G	N1-C6-O6	-5.38	116.67	119.90
1	X	1969	G	N3-C4-N9	5.37	129.22	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2567	G	C8-N9-C4	-5.37	104.25	106.40
1	X	31	C	C6-N1-C2	-5.37	118.15	120.30
1	X	1779	C	N1-C2-O2	-5.37	115.68	118.90
1	X	2800	C	C6-N1-C2	-5.37	118.15	120.30
1	X	2034	A	C2-N3-C4	5.37	113.28	110.60
1	X	762	A	N1-C6-N6	5.36	121.82	118.60
1	X	1801	C	C5-C6-N1	-5.36	118.32	121.00
1	X	1984	A	C6-N1-C2	-5.36	115.38	118.60
1	X	2699	G	C6-N1-C2	5.36	128.31	125.10
1	X	1339	U	N1-C2-O2	5.35	126.55	122.80
1	X	2591	C	N1-C2-O2	-5.35	115.69	118.90
1	X	2832	G	C5-N7-C8	-5.35	101.62	104.30
1	X	1275	A	C5-N7-C8	-5.35	101.23	103.90
1	X	1266	G	N1-C2-N3	5.34	127.11	123.90
1	X	1670	G	C2-N3-C4	-5.34	109.23	111.90
1	X	1298	G	C5-C6-O6	5.34	131.81	128.60
1	X	1312	G	N3-C2-N2	5.34	123.64	119.90
1	X	2656	G	N7-C8-N9	-5.34	110.43	113.10
1	X	832	A	C4-C5-N7	5.33	113.37	110.70
1	X	23	G	C5-C6-O6	5.33	131.80	128.60
1	X	2712	G	C8-N9-C4	5.33	108.53	106.40
1	X	527	C	C2-N1-C1'	5.33	124.66	118.80
1	X	570	G	N3-C2-N2	-5.32	116.17	119.90
1	X	1274	C	N1-C2-N3	-5.32	115.47	119.20
1	X	1442	C	N3-C4-C5	5.32	124.03	121.90
1	X	2478	C	N3-C4-N4	5.32	121.72	118.00
1	X	1246	G	N1-C6-O6	-5.32	116.71	119.90
1	X	1980	A	C4-C5-N7	-5.31	108.04	110.70
1	X	1652	G	N3-C4-C5	5.30	131.25	128.60
1	X	2519	C	N3-C4-C5	-5.30	119.78	121.90
1	X	346	C	C4-C5-C6	5.30	120.05	117.40
1	X	1685	A	N1-C6-N6	-5.30	115.42	118.60
1	X	1266	G	C5-C6-N1	-5.30	108.85	111.50
1	X	1321	A	N7-C8-N9	-5.30	111.15	113.80
1	X	754	G	N7-C8-N9	-5.30	110.45	113.10
1	X	465	C	C6-N1-C2	5.29	122.42	120.30
1	X	2478	C	C5-C6-N1	5.29	123.65	121.00
1	X	497	C	C6-N1-C2	5.29	122.42	120.30
1	X	2432	A	C8-N9-C4	-5.29	103.69	105.80
1	X	544	U	N1-C2-O2	5.28	126.50	122.80
1	X	949	G	C8-N9-C4	5.28	108.51	106.40
1	X	1939	U	N1-C2-O2	-5.28	119.11	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1763	G	N3-C2-N2	5.27	123.59	119.90
1	X	826	U	C5-C4-O4	5.27	129.06	125.90
1	X	699	G	C6-N1-C2	5.26	128.26	125.10
1	X	1742	G	C8-N9-C4	5.26	108.51	106.40
1	X	1665	C	N3-C4-C5	5.26	124.00	121.90
1	X	714	G	N1-C6-O6	-5.26	116.75	119.90
1	X	1211	G	N7-C8-N9	-5.26	110.47	113.10
1	X	796	A	C5-N7-C8	-5.25	101.27	103.90
1	X	714	G	C4-C5-N7	-5.25	108.70	110.80
13	K	10	LEU	CB-CG-CD2	5.25	119.93	111.00
1	X	2233	C	C5-C6-N1	-5.25	118.38	121.00
1	X	2809	A	C2-N3-C4	5.25	113.22	110.60
1	X	1468	A	C5-N7-C8	5.25	106.52	103.90
1	X	2717	G	N1-C6-O6	-5.25	116.75	119.90
1	X	772	G	C5-C6-N1	5.25	114.12	111.50
1	X	550	C	N1-C2-O2	-5.24	115.75	118.90
1	X	2616	U	C5-C4-O4	-5.24	122.75	125.90
1	X	1667	A	C8-N9-C4	5.24	107.90	105.80
1	X	568	G	C4-C5-N7	-5.24	108.71	110.80
1	X	2700	U	C5-C4-O4	5.24	129.04	125.90
1	X	2665	G	C4-C5-N7	-5.23	108.71	110.80
1	X	757	U	N3-C2-O2	-5.23	118.54	122.20
1	X	1662	G	C4-C5-N7	-5.23	108.71	110.80
1	X	2618	A	N9-C4-C5	5.23	107.89	105.80
1	X	2007	G	C5-N7-C8	5.23	106.91	104.30
13	K	5	LYS	CD-CE-NZ	5.23	123.72	111.70
1	X	2555	G	C8-N9-C4	5.22	108.49	106.40
1	X	1312	G	C6-C5-N7	-5.22	127.27	130.40
1	X	1931	G	N7-C8-N9	5.22	115.71	113.10
1	X	2667	C	N3-C2-O2	5.22	125.55	121.90
1	X	2807	U	N3-C4-O4	-5.22	115.75	119.40
1	X	537	C	C2-N3-C4	-5.21	117.29	119.90
1	X	1223	G	N1-C6-O6	5.21	123.03	119.90
1	X	1995	G	N1-C6-O6	-5.21	116.77	119.90
1	X	607	C	N3-C2-O2	-5.21	118.25	121.90
1	X	704	G	C5-C6-O6	5.21	131.72	128.60
1	X	2853	U	N1-C2-O2	5.21	126.45	122.80
1	X	1290	A	N1-C6-N6	5.21	121.72	118.60
1	X	2371	A	N9-C4-C5	5.20	107.88	105.80
1	X	2791	C	N3-C4-C5	5.20	123.98	121.90
1	X	121	G	C4-C5-N7	-5.20	108.72	110.80
1	X	1459	U	N3-C2-O2	5.19	125.83	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2748	C	N3-C2-O2	5.19	125.53	121.90
1	X	1662	G	C5-C6-O6	5.18	131.71	128.60
1	X	2815	C	N3-C4-C5	5.17	123.97	121.90
1	X	538	A	C5-C6-N6	-5.17	119.56	123.70
1	X	2766	U	N3-C4-O4	-5.16	115.79	119.40
1	X	2618	A	C6-N1-C2	-5.16	115.50	118.60
1	X	87	G	C8-N9-C4	-5.16	104.34	106.40
1	X	1743	C	C4-C5-C6	5.16	119.98	117.40
1	X	2683	C	C6-N1-C2	5.16	122.36	120.30
3	A	21	ASP	CB-CG-OD2	5.16	122.94	118.30
1	X	1665	C	C6-N1-C2	5.16	122.36	120.30
1	X	2796	A	C4-C5-C6	5.16	119.58	117.00
1	X	504	G	C2-N3-C4	-5.15	109.32	111.90
1	X	1278	A	C4-C5-C6	5.15	119.58	117.00
1	X	2824	C	C6-N1-C2	5.15	122.36	120.30
2	Y	84	G	C8-N9-C4	5.15	108.46	106.40
1	X	529	U	C6-N1-C2	-5.15	117.91	121.00
1	X	1694	A	C2-N3-C4	-5.15	108.03	110.60
1	X	1716	G	N1-C6-O6	-5.15	116.81	119.90
1	X	2848	A	C2-N3-C4	5.15	113.18	110.60
1	X	522	G	C5-N7-C8	-5.15	101.72	104.30
1	X	1992	G	C8-N9-C4	5.15	108.46	106.40
1	X	481	A	N1-C6-N6	5.15	121.69	118.60
1	X	1282	A	C2-N3-C4	-5.15	108.03	110.60
1	X	1764	A	N1-C2-N3	5.15	131.87	129.30
1	X	1993	G	N3-C4-C5	5.15	131.17	128.60
1	X	537	C	N3-C2-O2	-5.14	118.30	121.90
1	X	2592	U	C4-C5-C6	5.14	122.79	119.70
1	X	1260	A	N7-C8-N9	-5.14	111.23	113.80
1	X	544	U	N3-C4-O4	-5.14	115.80	119.40
1	X	1748	U	N1-C2-O2	-5.14	119.20	122.80
1	X	2594	U	C5-C6-N1	5.14	125.27	122.70
1	X	1632	A	C8-N9-C4	-5.14	103.75	105.80
1	X	1721	G	C8-N9-C4	5.14	108.45	106.40
1	X	1032	A	C8-N9-C4	-5.13	103.75	105.80
1	X	2224	U	C5-C4-O4	5.13	128.98	125.90
1	X	1467	U	C2-N1-C1'	5.13	123.85	117.70
1	X	2565	C	C6-N1-C2	-5.12	118.25	120.30
1	X	2611	A	N7-C8-N9	-5.12	111.24	113.80
1	X	2329	C	N3-C2-O2	5.12	125.48	121.90
1	X	1357	U	C5-C6-N1	-5.12	120.14	122.70
1	X	1998	A	N7-C8-N9	-5.11	111.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1678	G	C8-N9-C4	5.11	108.44	106.40
1	X	1770	U	N1-C2-N3	5.11	117.97	114.90
1	X	1822	C	C2-N3-C4	-5.11	117.35	119.90
1	X	2007	G	C5-C6-O6	5.10	131.66	128.60
1	X	459	A	P-O3'-C3'	5.10	125.82	119.70
1	X	1276	U	C5-C6-N1	-5.10	120.15	122.70
1	X	1305	C	C2-N3-C4	-5.10	117.35	119.90
1	X	1816	G	C4-C5-N7	-5.10	108.76	110.80
1	X	2520	A	C5-C6-N6	5.10	127.78	123.70
1	X	2815	C	C2-N3-C4	-5.10	117.35	119.90
1	X	2839	G	C8-N9-C4	5.10	108.44	106.40
1	X	2681	A	N9-C4-C5	-5.10	103.76	105.80
1	X	1281	A	N1-C2-N3	5.09	131.85	129.30
1	X	1302	C	C2-N1-C1'	-5.09	113.20	118.80
1	X	74	G	C8-N9-C4	5.09	108.44	106.40
1	X	345	U	N1-C2-O2	-5.09	119.24	122.80
1	X	2797	G	N3-C4-C5	-5.09	126.06	128.60
1	X	2590	U	C2-N3-C4	-5.09	123.95	127.00
1	X	1328	C	N3-C2-O2	-5.09	118.34	121.90
1	X	2623	A	N7-C8-N9	-5.08	111.26	113.80
1	X	2666	U	N1-C2-N3	5.08	117.95	114.90
1	X	2033	C	C6-N1-C2	-5.08	118.27	120.30
1	X	2680	U	N3-C2-O2	5.08	125.75	122.20
1	X	2764	U	C5-C6-N1	-5.08	120.16	122.70
1	X	29	U	C5-C6-N1	5.07	125.24	122.70
1	X	2008	C	N3-C4-C5	-5.07	119.87	121.90
1	X	330	C	C6-N1-C2	-5.07	118.27	120.30
1	X	695	G	N7-C8-N9	-5.07	110.57	113.10
1	X	1294	G	N1-C2-N3	5.07	126.94	123.90
1	X	2483	U	C6-N1-C2	-5.07	117.96	121.00
1	X	2556	A	N9-C4-C5	5.07	107.83	105.80
1	X	2748	C	N1-C2-O2	-5.07	115.86	118.90
1	X	190	A	C8-N9-C4	5.06	107.83	105.80
1	X	550	C	C6-N1-C2	5.06	122.33	120.30
1	X	1145	C	N1-C2-O2	-5.06	115.86	118.90
1	X	1999	U	N3-C2-O2	5.06	125.74	122.20
1	X	2408	G	C8-N9-C4	-5.06	104.38	106.40
1	X	2398	U	N3-C2-O2	-5.05	118.66	122.20
1	X	2658	A	C8-N9-C4	5.05	107.82	105.80
1	X	2760	G	N7-C8-N9	-5.05	110.57	113.10
1	X	1391	A	C8-N9-C4	5.05	107.82	105.80
2	Y	85	G	C2-N3-C4	-5.05	109.38	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1631	C	C5-C6-N1	-5.05	118.48	121.00
1	X	2804	G	C8-N9-C4	5.05	108.42	106.40
1	X	69	G	C8-N9-C4	5.05	108.42	106.40
15	M	71	ILE	CG1-CB-CG2	-5.05	100.30	111.40
1	X	2722	C	C6-N1-C2	5.04	122.32	120.30
1	X	196	A	C4-C5-N7	-5.04	108.18	110.70
1	X	1687	C	N3-C4-C5	-5.04	119.88	121.90
1	X	2260	C	N3-C4-C5	5.04	123.91	121.90
1	X	2556	A	C8-N9-C4	-5.04	103.79	105.80
1	X	340	G	N7-C8-N9	-5.03	110.58	113.10
1	X	1344	C	C5-C6-N1	-5.03	118.48	121.00
1	X	1614	C	N1-C2-O2	-5.03	115.88	118.90
1	X	2437	G	C5-C6-O6	-5.03	125.58	128.60
1	X	2005	U	C5-C6-N1	-5.03	120.19	122.70
1	X	122	G	C5-C6-N1	-5.03	108.99	111.50
1	X	542	A	C6-C5-N7	-5.03	128.78	132.30
1	X	1750	A	N1-C2-N3	5.03	131.81	129.30
1	X	1775	A	N7-C8-N9	-5.03	111.29	113.80
1	X	1979	C	N1-C2-O2	-5.03	115.88	118.90
1	X	1235	C	C6-N1-C2	5.02	122.31	120.30
1	X	2569	A	N7-C8-N9	-5.02	111.29	113.80
1	X	748	A	N1-C6-N6	5.02	121.61	118.60
1	X	966	A	C8-N9-C4	5.02	107.81	105.80
1	X	2375	G	C8-N9-C4	5.02	108.41	106.40
1	X	2545	A	N1-C6-N6	5.02	121.61	118.60
1	X	1652	G	N1-C6-O6	5.01	122.91	119.90
1	X	1660	G	C5-C6-O6	5.01	131.61	128.60
1	X	2542	U	C6-N1-C2	5.01	124.01	121.00
2	Y	20	A	C8-N9-C4	5.01	107.81	105.80
1	X	1274	C	C5-C4-N4	-5.01	116.69	120.20
1	X	2578	G	N3-C4-N9	5.01	129.01	126.00
1	X	2695	C	C6-N1-C2	-5.01	118.30	120.30
1	X	2762	G	N1-C6-O6	5.01	122.91	119.90
1	X	1339	U	C2-N1-C1'	5.01	123.71	117.70
1	X	490	A	N1-C6-N6	-5.01	115.60	118.60
1	X	1652	G	N9-C4-C5	-5.01	103.40	105.40
1	X	1687	C	C5-C6-N1	-5.01	118.50	121.00
1	X	1767	G	C5-C6-O6	-5.00	125.60	128.60
1	X	2798	A	C4-C5-N7	5.00	113.20	110.70

There are no chirality outliers.

There are no planarity outliers.

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	57035	0	28741	1817	0
2	Y	2561	0	1306	48	0
3	A	1920	0	1974	176	0
4	B	1539	0	1600	147	0
5	C	1481	0	1504	120	0
6	D	1400	0	1481	61	0
7	E	1286	0	1336	44	0
8	F	451	0	474	7	0
9	G	1114	0	1144	100	0
10	H	997	0	1046	98	0
11	I	1011	0	1047	98	0
12	J	1090	0	1125	78	0
13	K	878	0	930	80	0
14	L	779	0	820	72	0
15	M	871	0	894	99	0
16	N	978	0	1020	82	0
17	O	741	0	756	45	0
18	P	1004	0	1083	88	0
19	Q	726	0	753	50	0
20	R	825	0	881	69	0
21	S	1345	0	1372	43	0
22	T	556	0	579	38	0
23	U	552	0	604	48	0
24	V	525	0	546	29	0
25	W	424	0	470	17	0
26	Z	452	0	457	53	0
27	1	431	0	456	58	0
28	2	383	0	414	52	0
29	3	462	0	506	63	0
30	4	297	0	330	23	0
31	X	58	0	69	13	0
32	C	1	0	0	0	0
32	I	1	0	0	0	0
32	X	151	0	0	0	0
32	Y	1	0	0	0	0
33	A	1	0	0	0	0
33	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	X	37	0	0	0	0
33	Y	2	0	0	0	0
33	Z	1	0	0	0	0
34	M	1	0	0	0	0
34	X	14	0	0	0	0
All	All	84383	0	55718	3336	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 24.

All (3336) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2044:G:OP1	5:C:62:LYS:HG3	1.36	1.18
15:M:28:ARG:HB2	15:M:29:PRO:HD3	1.29	1.14
9:G:103:TYR:HB3	9:G:107:GLN:HE21	1.14	1.12
4:B:9:ILE:HD11	4:B:27:LEU:HB2	1.32	1.10
4:B:116:VAL:HG22	4:B:136:ARG:NE	1.69	1.05
9:G:67:ARG:HB3	9:G:70:PHE:HA	1.39	1.05
10:H:83:ARG:HD2	10:H:89:ILE:HD11	1.38	1.05
28:2:10:ARG:H	28:2:10:ARG:HD2	1.19	1.05
9:G:100:TYR:HB2	9:G:116:ARG:HH11	1.20	1.04
4:B:116:VAL:HG22	4:B:136:ARG:HE	1.21	1.03
23:U:17:SER:HB2	23:U:44:ALA:HA	1.36	1.03
5:C:176:ASN:HD21	5:C:178:TYR:HB3	1.22	1.03
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.71	1.02
1:X:591:G:H2'	1:X:592:G:C8	1.94	1.02
3:A:96:LEU:HD12	3:A:106:ILE:HD12	1.43	1.00
1:X:552:C:H2'	1:X:553:C:H5"	1.41	1.00
3:A:244:GLY:H	3:A:245:ARG:NH1	1.60	1.00
16:N:50:ARG:HA	16:N:53:LYS:HE2	1.43	1.00
6:D:38:GLU:HB3	6:D:87:ILE:HB	1.42	0.99
2:Y:17:A:H1'	2:Y:112:A:C8	1.97	0.99
9:G:106:TYR:CE2	9:G:108:GLY:HA3	1.99	0.98
1:X:2797:G:OP2	13:K:3:HIS:CE1	2.16	0.97
14:L:31:VAL:HG23	14:L:38:ILE:HD13	1.46	0.97
3:A:49:ARG:H	3:A:49:ARG:HD2	1.29	0.97
29:3:13:ARG:HH11	29:3:25:PHE:HB2	1.30	0.96
1:X:1466:C:H2'	1:X:1467:U:O4'	1.67	0.95
4:B:14:ILE:HG12	15:M:20:HIS:CD2	2.02	0.95
9:G:132:PHE:HD2	9:G:145:HIS:CD2	1.84	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:20:ARG:HD3	23:U:43:ARG:HH22	1.30	0.94
1:X:2592:U:H2'	26:Z:5:PRO:HG2	1.48	0.93
5:C:176:ASN:HD22	5:C:179:ASP:H	1.10	0.93
1:X:2736:U:H3	1:X:2738:A:H62	1.05	0.93
1:X:540:G:H2'	1:X:542:A:H2	1.31	0.93
1:X:760:U:C6	26:Z:3:LYS:HE2	2.04	0.92
1:X:2170:C:H3'	1:X:2171:U:H5"	1.49	0.92
1:X:2757:G:H5"	1:X:2758:A:H5'	1.49	0.91
9:G:132:PHE:CD2	9:G:145:HIS:CD2	2.57	0.91
4:B:14:ILE:HA	15:M:20:HIS:HD2	1.34	0.91
3:A:44:ARG:HD2	3:A:44:ARG:N	1.83	0.91
4:B:110:GLY:HA2	4:B:161:GLY:HA3	1.52	0.91
1:X:2044:G:OP1	5:C:62:LYS:CG	2.18	0.91
22:T:12:ASN:HB3	22:T:14:ARG:HG2	1.51	0.91
1:X:225:G:C2	1:X:2410:U:H4'	2.05	0.91
31:X:2881:LMA:H37B	31:X:2881:LMA:H35	1.52	0.91
13:K:45:ARG:HG3	13:K:95:THR:HG21	1.54	0.90
23:U:49:LYS:HB3	23:U:61:TRP:CE3	2.05	0.90
5:C:26:VAL:HG22	11:I:18:ARG:HH12	1.35	0.90
1:X:2426:G:H3'	1:X:2479:U:OP2	1.72	0.90
1:X:2447:G:HO2'	1:X:2448:A:H8	0.91	0.90
15:M:11:GLU:HG3	15:M:14:ARG:HH11	1.36	0.90
1:X:635:C:H2'	1:X:636:G:H5"	1.50	0.90
9:G:103:TYR:HB3	9:G:107:GLN:NE2	1.86	0.89
20:R:15:HIS:HD1	20:R:16:PHE:HD2	1.19	0.89
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.53	0.89
20:R:18:LYS:H	20:R:18:LYS:HD3	1.36	0.89
20:R:22:VAL:HG11	20:R:80:LYS:HE3	1.54	0.89
2:Y:119:G:H4'	14:L:57:ALA:HB3	1.55	0.89
18:P:66:GLU:HB3	18:P:67:PRO:HD3	1.53	0.88
1:X:347:C:H4'	20:R:15:HIS:CD2	2.08	0.88
1:X:870:C:H1'	22:T:26:PHE:HE2	1.39	0.88
15:M:33:VAL:HG22	15:M:51:GLU:HB2	1.53	0.88
27:1:34:LYS:HE3	27:1:34:LYS:HA	1.56	0.88
1:X:1296:G:H22	1:X:1299:A:H5"	1.39	0.87
1:X:2204:A:H4'	1:X:2205:C:O5'	1.71	0.87
7:E:103:LEU:HD21	7:E:131:ILE:HD13	1.55	0.87
12:J:15:ARG:HD3	12:J:73:LYS:HG3	1.56	0.87
13:K:84:ALA:HB3	13:K:85:PRO:HD3	1.55	0.87
3:A:44:ARG:HD2	3:A:44:ARG:H	1.34	0.87
2:Y:59:A:H1'	6:D:27:ALA:HB2	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1816:G:OP1	3:A:53:ARG:HD3	1.75	0.86
1:X:2811:G:H2'	1:X:2812:A:C8	2.11	0.86
7:E:105:MET:HB2	7:E:113:VAL:HB	1.57	0.86
13:K:100:VAL:HG12	13:K:101:GLY:N	1.90	0.86
1:X:870:C:H4'	22:T:23:VAL:HG21	1.56	0.86
1:X:1086:C:H3'	1:X:1087:C:H5"	1.57	0.86
2:Y:33:C:H42	2:Y:53:G:H1	1.22	0.86
1:X:1790:G:H4'	1:X:1791:C:O5'	1.77	0.85
9:G:106:TYR:CE2	9:G:108:GLY:CA	2.59	0.85
10:H:25:LEU:HD11	10:H:52:VAL:HG23	1.55	0.85
1:X:1067:G:H21	1:X:1114:A:H62	1.21	0.85
1:X:313:U:H2'	1:X:314:G:H8	1.39	0.85
4:B:76:ARG:NH1	15:M:4:HIS:HB2	1.91	0.85
5:C:163:ASN:HD21	5:C:167:VAL:H	1.21	0.85
1:X:2598:C:O2'	1:X:2599:U:H5'	1.77	0.85
28:2:37:LYS:O	28:2:40:HIS:HE1	1.59	0.85
12:J:42:TRP:HB3	12:J:95:VAL:HG11	1.55	0.84
31:X:2881:LMA:H32	31:X:2881:LMA:O53	1.76	0.84
11:I:31:GLY:O	11:I:32:ARG:HG3	1.77	0.84
1:X:347:C:H4'	20:R:15:HIS:HD2	1.38	0.84
20:R:15:HIS:ND1	20:R:16:PHE:HD2	1.75	0.84
25:W:46:THR:HG22	25:W:47:VAL:HG13	1.60	0.84
1:X:918:A:H2'	1:X:919:U:H5"	1.60	0.84
3:A:173:TYR:HA	3:A:187:HIS:HA	1.60	0.84
1:X:1811:A:H4'	1:X:1812:U:O5'	1.78	0.83
3:A:43:GLY:C	3:A:44:ARG:HH11	1.81	0.83
9:G:162:LYS:H	9:G:163:PRO:HD2	1.43	0.83
1:X:504:G:H4'	18:P:27:VAL:HG13	1.60	0.83
1:X:1469:U:H5'	1:X:1470:G:OP2	1.77	0.83
13:K:49:GLU:OE1	13:K:95:THR:HG22	1.77	0.83
16:N:66:ASN:HB2	16:N:70:ARG:HH12	1.43	0.83
10:H:2:ILE:HB	10:H:45:ALA:HB3	1.60	0.83
4:B:131:SER:HB2	4:B:134:TRP:CD1	2.12	0.83
18:P:85:MET:HE3	18:P:130:GLU:HG3	1.61	0.82
1:X:165:G:H1	1:X:185:C:H42	1.27	0.82
1:X:2266:A:O2'	1:X:2267:A:H2'	1.78	0.82
13:K:98:LEU:HD23	26:Z:45:ILE:HD11	1.59	0.82
1:X:1147:G:H2'	1:X:1148:G:H8	1.45	0.82
1:X:1631:C:H1'	18:P:108:PRO:HG2	1.59	0.82
4:B:146:THR:HB	4:B:147:PRO:HD2	1.59	0.82
20:R:22:VAL:HG13	20:R:81:VAL:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2194:A:H3'	1:X:2195:C:H5"	1.60	0.82
1:X:595:A:H5'	5:C:83:ALA:HB3	1.62	0.81
1:X:2796:A:P	13:K:3:HIS:HE2	2.03	0.81
18:P:95:ALA:HB2	18:P:126:ILE:HD13	1.61	0.81
26:Z:42:SER:O	26:Z:44:HIS:HD2	1.63	0.81
1:X:2200:G:H2'	1:X:2201:G:C8	2.15	0.81
1:X:2289:A:H2	6:D:79:LEU:HD11	1.44	0.81
23:U:20:ARG:HD3	23:U:43:ARG:NH2	1.94	0.81
3:A:80:VAL:HB	3:A:115:GLY:H	1.46	0.81
27:1:9:ILE:HA	27:1:28:ARG:HA	1.62	0.80
1:X:938:G:O2'	1:X:939:C:H5'	1.82	0.80
3:A:25:LEU:CB	3:A:206:VAL:HG22	2.12	0.80
14:L:37:HIS:CE1	14:L:57:ALA:HB2	2.16	0.80
1:X:540:G:H2'	1:X:542:A:C2	2.16	0.80
1:X:408:U:H2'	1:X:409:G:C8	2.16	0.80
1:X:2797:G:OP2	13:K:3:HIS:HE1	1.60	0.80
18:P:103:LEU:HB2	18:P:119:LYS:HB2	1.62	0.80
20:R:90:LYS:HB2	20:R:108:VAL:HG21	1.64	0.80
1:X:1053:G:H4'	1:X:1054:C:OP1	1.80	0.80
28:2:43:THR:O	28:2:43:THR:HG22	1.78	0.79
1:X:1016:C:O2'	9:G:56:THR:HG21	1.81	0.79
15:M:99:VAL:HG21	15:M:104:LEU:HD21	1.62	0.79
4:B:174:GLU:HB3	4:B:183:LEU:HD12	1.64	0.79
1:X:37:C:H1'	5:C:44:SER:OG	1.83	0.79
10:H:13:ASN:HD21	10:H:109:ARG:HG2	1.48	0.79
10:H:116:ARG:HD2	15:M:38:LYS:NZ	1.98	0.79
1:X:2861:A:O2'	26:Z:31:THR:HG23	1.83	0.79
1:X:666:U:H2'	1:X:667:U:H5"	1.64	0.79
1:X:1630:A:N1	18:P:114:ALA:HB2	1.98	0.79
27:1:39:LYS:NZ	27:1:47:HIS:HA	1.98	0.79
13:K:49:GLU:O	13:K:52:ILE:HG12	1.83	0.79
18:P:41:VAL:O	18:P:44:VAL:HG22	1.82	0.79
22:T:43:THR:HG22	22:T:43:THR:O	1.82	0.79
1:X:1142:G:N3	9:G:103:TYR:HD2	1.80	0.78
5:C:154:ASP:O	5:C:157:THR:HG22	1.83	0.78
3:A:69:LYS:HD3	3:A:69:LYS:H	1.48	0.78
16:N:66:ASN:HB2	16:N:70:ARG:NH1	1.98	0.78
1:X:824:U:C2'	11:I:30:ALA:HB2	2.14	0.78
1:X:2672:U:H2'	1:X:2673:G:H8	1.49	0.78
1:X:1404:C:H5'	1:X:1405:A:OP2	1.84	0.78
10:H:27:SER:HA	10:H:50:ILE:HD12	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:168:A:H2'	1:X:169:C:C6	2.19	0.78
1:X:469:G:H5'	28:2:39:ARG:HB2	1.66	0.77
1:X:2796:A:OP2	13:K:3:HIS:NE2	2.16	0.77
27:1:14:SER:HB2	27:1:22:TYR:HA	1.67	0.77
28:2:37:LYS:O	28:2:40:HIS:CE1	2.37	0.77
1:X:1976:U:H4'	4:B:128:SER:OG	1.83	0.77
1:X:317:U:H2'	1:X:318:G:H5'	1.65	0.77
10:H:76:ARG:O	10:H:94:ASN:HA	1.84	0.77
1:X:2659:C:H5'	4:B:189:PRO:HA	1.65	0.77
1:X:313:U:H2'	1:X:314:G:C8	2.20	0.77
3:A:61:ARG:HD3	3:A:88:ASN:OD1	1.85	0.77
18:P:87:GLU:HA	18:P:90:LEU:HG	1.67	0.77
1:X:1584:G:H5"	3:A:62:LEU:HG	1.67	0.77
5:C:5:ASN:HA	5:C:118:VAL:HG23	1.67	0.77
14:L:89:PHE:HB3	14:L:91:ARG:NH2	1.99	0.77
27:1:39:LYS:CE	27:1:47:HIS:HA	2.15	0.76
1:X:492:G:H22	1:X:519:C:H42	1.32	0.76
16:N:6:THR:O	16:N:9:VAL:HG23	1.84	0.76
4:B:78:LEU:O	4:B:79:ARG:HD3	1.86	0.76
10:H:10:VAL:HG23	10:H:17:ARG:O	1.84	0.76
11:I:74:VAL:HG13	11:I:109:LEU:HD12	1.68	0.76
15:M:28:ARG:CB	15:M:29:PRO:HD3	2.11	0.76
1:X:2495:G:O2'	1:X:2496:C:H5'	1.85	0.76
5:C:162:ARG:HD2	5:C:162:ARG:C	2.05	0.76
13:K:98:LEU:HD21	26:Z:56:GLN:HG2	1.67	0.76
27:1:29:ARG:HA	27:1:33:ALA:CB	2.16	0.76
19:Q:53:ILE:HD13	19:Q:80:VAL:HG12	1.65	0.76
2:Y:51:G:H2'	2:Y:52:G:C8	2.21	0.76
3:A:143:VAL:HG12	3:A:194:ILE:HA	1.67	0.76
1:X:824:U:H2'	11:I:30:ALA:HB2	1.66	0.75
1:X:2590:U:C5	26:Z:4:HIS:NE2	2.53	0.75
27:1:8:ILE:HD13	27:1:8:ILE:H	1.49	0.75
1:X:1314:A:O2'	1:X:1315:A:H3'	1.86	0.75
27:1:14:SER:CB	27:1:23:THR:H	1.99	0.75
1:X:542:A:H2'	16:N:28:ARG:NE	2.01	0.75
1:X:1441:A:H4'	1:X:1442:C:O5'	1.84	0.75
10:H:99:ILE:HD12	10:H:103:GLY:HA2	1.67	0.75
1:X:1016:C:HO2'	1:X:1023:U:H5	1.34	0.75
3:A:71:ARG:HG2	3:A:191:TYR:CE1	2.22	0.75
5:C:162:ARG:HD2	5:C:162:ARG:O	1.86	0.75
11:I:43:ALA:O	11:I:45:LYS:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1048:U:H3	1:X:1129:A:H61	1.33	0.75
1:X:2811:G:H2'	1:X:2812:A:H8	1.49	0.75
14:L:38:ILE:HD12	14:L:39:TYR:H	1.51	0.75
18:P:59:PHE:HD1	26:Z:30:LEU:HD11	1.52	0.75
27:1:29:ARG:HA	27:1:33:ALA:HB2	1.67	0.75
1:X:128:C:H2'	1:X:129:A:H5"	1.68	0.75
21:S:51:LEU:HD23	21:S:51:LEU:H	1.51	0.75
1:X:1673:C:H2'	1:X:1674:C:H6	1.52	0.74
2:Y:51:G:H2'	2:Y:52:G:H8	1.51	0.74
12:J:99:LYS:HE3	12:J:100:PRO:HD2	1.69	0.74
4:B:11:MET:HG2	4:B:24:THR:OG1	1.87	0.74
1:X:2484:G:O2'	1:X:2485:U:H5"	1.87	0.74
1:X:1444:C:H42	1:X:1579:G:H1	1.33	0.74
3:A:209:LYS:HA	3:A:209:LYS:HE3	1.68	0.74
21:S:100:THR:HG23	21:S:138:VAL:HG11	1.69	0.74
1:X:1173:G:H4'	17:O:22:VAL:HG22	1.70	0.74
4:B:14:ILE:HD12	4:B:23:VAL:HG21	1.70	0.74
13:K:28:LEU:C	13:K:28:LEU:HD23	2.08	0.74
1:X:754:G:H2'	1:X:755:C:H6	1.52	0.74
19:Q:62:ARG:O	19:Q:63:LYS:HB3	1.88	0.74
1:X:2245:A:H4'	1:X:2246:A:N3	2.02	0.74
29:3:30:ARG:HH21	29:3:31:HIS:CE1	2.06	0.74
29:3:60:LEU:HD12	29:3:63:PRO:HG2	1.69	0.74
1:X:161:U:H4'	1:X:194:G:H21	1.51	0.73
1:X:2590:U:C5	26:Z:4:HIS:CE1	2.76	0.73
15:M:32:THR:O	15:M:51:GLU:HA	1.89	0.73
1:X:552:C:C2'	1:X:553:C:H5"	2.17	0.73
1:X:2660:C:H42	1:X:2707:G:H1	1.37	0.73
15:M:104:LEU:HA	15:M:106:TYR:CE2	2.24	0.73
26:Z:6:VAL:HG13	26:Z:7:PRO:HD2	1.70	0.73
3:A:54:PHE:O	3:A:55:ILE:HB	1.87	0.73
3:A:245:ARG:C	3:A:253:LYS:HE2	2.09	0.73
29:3:13:ARG:NH1	29:3:25:PHE:HB2	2.03	0.73
6:D:60:ILE:HG13	6:D:61:THR:HG23	1.71	0.73
13:K:87:TYR:HE1	13:K:94:TYR:HD1	1.36	0.73
1:X:590:C:H2'	1:X:591:G:H8	1.54	0.73
26:Z:52:TYR:O	26:Z:53:ASP:HB2	1.89	0.73
1:X:1336:G:H2'	1:X:1337:G:H5'	1.69	0.73
1:X:1542:G:H22	1:X:1562:G:H1	1.37	0.73
1:X:73:A:H5"	1:X:74:G:O4'	1.89	0.72
18:P:37:LYS:HE2	18:P:64:ALA:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:51:ILE:HG23	23:U:59:THR:HG22	1.71	0.72
29:3:13:ARG:HD2	29:3:25:PHE:N	2.04	0.72
18:P:25:PHE:HD1	18:P:127:ILE:HD11	1.54	0.72
1:X:177:U:H3'	23:U:40:ARG:HH21	1.53	0.72
1:X:2734:U:H4'	30:4:26:ILE:HD13	1.70	0.72
14:L:38:ILE:HD11	14:L:40:ALA:H	1.53	0.72
1:X:394:U:OP1	23:U:19:ILE:HD11	1.89	0.72
1:X:1277:G:OP1	26:Z:19:ARG:NH2	2.22	0.72
1:X:1278:A:H2	1:X:1997:A:H62	1.37	0.72
11:I:58:ALA:HA	29:3:12:ARG:HH21	1.54	0.72
20:R:29:HIS:CD2	20:R:51:VAL:HG22	2.24	0.72
1:X:540:G:C2'	1:X:542:A:H2	2.02	0.72
1:X:797:A:C5	3:A:230:VAL:HG21	2.24	0.72
1:X:2825:A:H2'	1:X:2825:A:N3	2.04	0.72
1:X:73:A:H3'	1:X:74:G:H5'	1.72	0.72
1:X:654:A:H3'	1:X:654:A:N3	2.04	0.72
1:X:1656:U:C2'	1:X:1657:A:H5"	2.20	0.72
1:X:2218:G:H5'	3:A:250:PRO:HD3	1.70	0.72
26:Z:58:LEU:H	26:Z:58:LEU:HD12	1.54	0.72
9:G:103:TYR:CB	9:G:107:GLN:HE21	1.99	0.72
11:I:49:PHE:HD1	11:I:50:GLU:H	1.38	0.72
24:V:42:ARG:O	24:V:46:LEU:HG	1.90	0.72
1:X:2260:C:O2'	1:X:2261:G:H5'	1.89	0.72
1:X:1884:A:O2'	3:A:245:ARG:HG2	1.90	0.71
1:X:2284:U:H4'	6:D:133:LYS:HG2	1.70	0.71
1:X:2736:U:H5"	30:4:19:ARG:HG2	1.72	0.71
1:X:635:C:C2'	1:X:636:G:H5"	2.20	0.71
1:X:1714:A:H5"	1:X:1715:A:H2'	1.71	0.71
3:A:253:LYS:H	3:A:254:PRO:HD2	1.55	0.71
6:D:4:LEU:HG	6:D:5:LYS:H	1.54	0.71
1:X:841:G:H2'	1:X:842:A:C8	2.26	0.71
1:X:1688:U:HO2'	1:X:1690:U:H5	1.38	0.71
1:X:2291:U:O2'	6:D:86:GLY:HA3	1.91	0.71
16:N:99:ALA:HB2	16:N:106:PHE:CD1	2.26	0.71
1:X:1745:C:H2'	1:X:1746:A:O4'	1.91	0.71
13:K:45:ARG:HG3	13:K:95:THR:CG2	2.21	0.71
28:2:43:THR:O	28:2:43:THR:CG2	2.38	0.71
1:X:2704:U:H2'	1:X:2705:A:C2	2.26	0.71
3:A:45:ASN:HB3	3:A:50:ILE:HA	1.71	0.71
4:B:144:ARG:HG2	4:B:145:LYS:H	1.55	0.71
1:X:504:G:H4'	18:P:27:VAL:CG1	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:28:LEU:HD23	13:K:28:LEU:O	1.90	0.71
1:X:839:U:H5"	1:X:2408:G:OP2	1.91	0.70
1:X:870:C:H1'	22:T:26:PHE:CE2	2.23	0.70
1:X:1147:G:H2'	1:X:1148:G:C8	2.26	0.70
9:G:132:PHE:HB2	9:G:145:HIS:CD2	2.26	0.70
10:H:23:ARG:NH2	10:H:23:ARG:HB3	2.06	0.70
1:X:2048:C:H1'	1:X:2428:U:H3	1.56	0.70
9:G:106:TYR:HE2	9:G:108:GLY:HA3	1.54	0.70
25:W:4:LYS:HG3	25:W:52:GLU:HB3	1.73	0.70
1:X:557:U:H4'	1:X:558:G:O4'	1.92	0.70
1:X:2051:U:H3	1:X:2409:A:H62	1.38	0.70
1:X:2781:G:H2'	1:X:2782:G:H5"	1.72	0.70
15:M:34:ARG:HH21	15:M:91:VAL:HG21	1.55	0.70
1:X:590:C:H2'	1:X:591:G:C8	2.27	0.70
15:M:104:LEU:HD23	15:M:106:TYR:HE2	1.57	0.70
16:N:17:VAL:HG21	16:N:32:TYR:HE1	1.55	0.70
1:X:242:A:O2'	1:X:243:G:H4'	1.90	0.70
1:X:2194:A:C3'	1:X:2195:C:H5"	2.21	0.70
1:X:2592:U:H2'	26:Z:5:PRO:CG	2.21	0.70
19:Q:12:ILE:H	19:Q:12:ILE:HD13	1.55	0.70
1:X:1174:G:N2	1:X:1175:A:C4	2.60	0.70
14:L:38:ILE:CD1	14:L:40:ALA:H	2.05	0.70
4:B:116:VAL:HG13	4:B:136:ARG:HH21	1.57	0.70
10:H:41:ASN:O	10:H:42:LYS:O	2.10	0.70
1:X:595:A:H5'	5:C:83:ALA:CB	2.22	0.69
1:X:2756:A:H4'	1:X:2757:G:O5'	1.91	0.69
2:Y:39:C:H5'	2:Y:40:C:OP2	1.92	0.69
20:R:23:ILE:HG22	20:R:33:THR:HB	1.73	0.69
15:M:34:ARG:CZ	15:M:88:VAL:HG11	2.22	0.69
1:X:1043:A:H5'	30:4:7:VAL:O	1.92	0.69
10:H:110:VAL:HG23	10:H:129:LEU:HB2	1.74	0.69
19:Q:63:LYS:HD3	19:Q:69:ILE:HA	1.73	0.69
1:X:183:U:H6	1:X:183:U:O5'	1.76	0.69
1:X:539:A:C5	1:X:2025:A:C2	2.80	0.69
1:X:564:U:H2'	1:X:565:A:C8	2.27	0.69
1:X:2324:G:N3	1:X:2360:C:H2'	2.07	0.69
1:X:45:C:OP2	1:X:192:G:H2'	1.93	0.69
3:A:44:ARG:N	3:A:44:ARG:HH11	1.91	0.69
5:C:153:ASP:O	5:C:154:ASP:HB3	1.91	0.69
1:X:543:G:H5'	16:N:24:PHE:CE1	2.28	0.69
1:X:591:G:H2'	1:X:592:G:H8	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1148:G:H5”	1:X:1149:G:OP2	1.93	0.69
1:X:2240:C:O2’	1:X:2241:U:H5’	1.92	0.69
1:X:538:A:C4’	1:X:539:A:OP1	2.41	0.69
1:X:538:A:H2’	1:X:538:A:N3	2.06	0.69
1:X:1656:U:H2’	1:X:1657:A:H5”	1.75	0.69
1:X:2660:C:N4	1:X:2707:G:H1	1.91	0.69
9:G:70:PHE:HB3	16:N:64:ARG:HG2	1.74	0.69
10:H:116:ARG:CZ	15:M:38:LYS:HE3	2.23	0.69
16:N:101:ARG:O	16:N:103:PRO:HD3	1.93	0.69
24:V:18:ILE:HG22	24:V:22:LYS:HE2	1.74	0.69
1:X:971:A:H61	12:J:83:ARG:HH22	1.40	0.69
1:X:2293:G:H5”	6:D:35:VAL:HG21	1.75	0.69
3:A:71:ARG:HH22	3:A:150:PRO:HA	1.57	0.69
1:X:317:U:C2’	1:X:318:G:H5’	2.22	0.69
1:X:2670:C:H4’	1:X:2846:G:O2’	1.93	0.69
4:B:60:ASN:HB3	4:B:62:PRO:HD2	1.74	0.69
14:L:89:PHE:HZ	14:L:103:LEU:HD22	1.58	0.69
1:X:1442:C:O2’	1:X:1585:A:OP2	2.08	0.68
4:B:131:SER:HB2	4:B:134:TRP:NE1	2.08	0.68
10:H:47:VAL:HA	10:H:74:VAL:HG12	1.75	0.68
15:M:39:VAL:HG12	15:M:45:THR:HG23	1.75	0.68
1:X:239:A:H5”	1:X:621:U:H5’	1.75	0.68
1:X:491:A:H4’	20:R:55:THR:HB	1.74	0.68
1:X:1166:A:H5”	16:N:55:ARG:HD3	1.74	0.68
1:X:2293:G:H5’	6:D:35:VAL:HG11	1.76	0.68
1:X:342:G:H4’	1:X:343:A:OP2	1.92	0.68
3:A:218:ARG:HG2	3:A:219:LYS:H	1.58	0.68
1:X:1096:A:H4’	1:X:1097:A:OP1	1.93	0.68
4:B:155:ARG:HH11	4:B:155:ARG:HG3	1.57	0.68
12:J:12:LYS:O	12:J:13:GLN:HB2	1.93	0.68
10:H:75:VAL:HG12	10:H:118:LEU:HD21	1.76	0.68
1:X:919:U:H2’	1:X:920:G:H8	1.59	0.68
1:X:1493:A:H2’	1:X:1494:G:O4’	1.94	0.68
16:N:72:HIS:HD2	16:N:110:VAL:HG21	1.58	0.68
28:2:42:LEU:N	28:2:42:LEU:HD12	2.09	0.68
1:X:337:G:HO2’	20:R:9:HIS:HD1	1.42	0.68
16:N:49:ASP:O	16:N:53:LYS:HG2	1.94	0.67
30:4:19:ARG:HD2	30:4:24:LEU:HD22	1.75	0.67
1:X:597:U:H2’	1:X:598:U:C6	2.29	0.67
1:X:2447:G:O2’	1:X:2448:A:H8	1.72	0.67
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:51:LEU:HD21	13:K:70:ILE:HD11	1.74	0.67
1:X:408:U:H2'	1:X:409:G:H8	1.59	0.67
1:X:854:G:H1	1:X:948:C:H42	1.41	0.67
1:X:1976:U:H4'	4:B:128:SER:CB	2.24	0.67
1:X:1988:A:H5"	1:X:1989:C:OP2	1.94	0.67
4:B:183:LEU:HD21	15:M:16:ILE:HG21	1.76	0.67
9:G:84:ASN:O	9:G:152:ALA:HA	1.94	0.67
11:I:61:PRO:HD3	29:3:27:SER:HB3	1.75	0.67
1:X:2551:A:N7	4:B:145:LYS:HB2	2.08	0.67
5:C:176:ASN:ND2	5:C:178:TYR:HB3	2.03	0.67
13:K:87:TYR:HE1	13:K:94:TYR:CD1	2.12	0.67
1:X:494:A:C8	20:R:56:LYS:HD2	2.30	0.67
12:J:64:LYS:NZ	12:J:110:VAL:HG13	2.10	0.67
12:J:66:TYR:HB2	12:J:106:GLU:HG2	1.75	0.67
17:O:34:GLU:HB2	17:O:56:VAL:CG2	2.24	0.67
1:X:1357:U:H4'	1:X:1397:A:C6	2.30	0.67
1:X:923:A:H5"	1:X:924:C:H5"	1.74	0.67
15:M:39:VAL:HG12	15:M:45:THR:OG1	1.93	0.67
23:U:23:LYS:HB2	23:U:35:THR:HG23	1.76	0.67
7:E:146:ALA:O	7:E:150:LYS:HG3	1.95	0.67
23:U:22:GLY:HA3	23:U:39:LYS:HG3	1.77	0.67
1:X:652:C:H42	1:X:657:A:H61	1.41	0.67
1:X:1991:C:H2'	1:X:1992:G:H8	1.60	0.67
1:X:38:G:H4'	1:X:39:C:OP1	1.95	0.66
1:X:538:A:H3'	9:G:142:ARG:HH12	1.57	0.66
1:X:1141:U:C4	4:B:147:PRO:HG3	2.29	0.66
1:X:1978:U:C2	1:X:1979:C:C5	2.83	0.66
1:X:2200:G:H2'	1:X:2201:G:H8	1.58	0.66
3:A:78:ALA:HB2	3:A:98:TYR:HD1	1.59	0.66
4:B:120:TRP:CD2	4:B:155:ARG:HD2	2.30	0.66
12:J:40:PRO:HB3	12:J:99:LYS:HZ2	1.60	0.66
19:Q:27:PHE:CZ	19:Q:42:ILE:HD13	2.30	0.66
20:R:75:ALA:O	20:R:76:LEU:HD23	1.95	0.66
1:X:1563:U:H2'	1:X:1564:U:C6	2.31	0.66
5:C:151:VAL:HG12	5:C:173:ALA:HA	1.76	0.66
6:D:65:PRO:HB3	6:D:89:VAL:HG22	1.77	0.66
9:G:162:LYS:N	9:G:163:PRO:HD2	2.09	0.66
10:H:1:MET:HB3	10:H:44:TYR:HB3	1.75	0.66
19:Q:10:PRO:HD3	24:V:30:PHE:CD2	2.30	0.66
1:X:2043:A:H62	5:C:68:ARG:NH1	1.93	0.66
1:X:2675:U:H2'	1:X:2676:G:C8	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:246:VAL:HG12	3:A:252:GLY:N	2.11	0.66
18:P:67:PRO:O	18:P:71:VAL:HG23	1.95	0.66
1:X:1107:A:H3'	1:X:1108:U:H5"	1.78	0.66
1:X:1941:C:O2'	1:X:1942:G:H5'	1.96	0.66
29:3:13:ARG:HD2	29:3:25:PHE:H	1.60	0.66
29:3:46:LYS:HA	29:3:46:LYS:HE3	1.77	0.66
1:X:826:U:H2'	1:X:827:C:C6	2.29	0.66
1:X:984:A:C2	1:X:1201:G:N2	2.64	0.66
1:X:2409:A:H4'	1:X:2410:U:OP1	1.96	0.66
1:X:2543:A:C2	1:X:2626:U:H4'	2.30	0.66
5:C:163:ASN:HD21	5:C:167:VAL:N	1.93	0.66
15:M:66:PHE:HD2	15:M:83:PHE:CE1	2.14	0.66
16:N:61:TRP:O	16:N:65:ILE:HG13	1.96	0.66
1:X:1343:C:O2'	1:X:1344:C:H5'	1.96	0.66
1:X:1469:U:H5	13:K:64:ARG:HH21	1.42	0.66
1:X:1683:G:O2'	1:X:1684:G:H5'	1.95	0.66
1:X:1968:G:H2'	1:X:1969:G:H8	1.59	0.66
3:A:244:GLY:N	3:A:245:ARG:NH1	2.41	0.66
4:B:76:ARG:HH12	15:M:4:HIS:HB2	1.61	0.66
1:X:1300:A:H5'	13:K:103:ARG:HD2	1.78	0.66
1:X:1468:A:C8	1:X:1468:A:OP2	2.49	0.66
22:T:21:LEU:HD21	22:T:41:ARG:HE	1.59	0.66
22:T:23:VAL:HG13	22:T:38:VAL:HG22	1.77	0.66
29:3:9:MET:HG3	29:3:60:LEU:HD22	1.77	0.66
1:X:477:A:OP1	28:2:34:ARG:NH2	2.29	0.66
1:X:879:A:H2'	1:X:879:A:N3	2.10	0.66
4:B:13:GLN:O	4:B:14:ILE:HG13	1.96	0.66
27:1:39:LYS:HE2	27:1:47:HIS:HA	1.75	0.66
9:G:132:PHE:CD2	9:G:145:HIS:CG	2.84	0.65
12:J:116:LYS:O	12:J:120:ARG:HB2	1.95	0.65
15:M:37:THR:CG2	15:M:39:VAL:HG13	2.26	0.65
1:X:1053:G:C4'	1:X:1054:C:OP1	2.43	0.65
1:X:1128:G:H2'	1:X:1129:A:H5"	1.78	0.65
1:X:1938:U:H1'	1:X:1939:U:OP1	1.97	0.65
1:X:2705:A:O4'	1:X:2705:A:N3	2.28	0.65
3:A:219:LYS:HD2	3:A:219:LYS:C	2.17	0.65
5:C:46:ARG:HB3	5:C:51:VAL:HG23	1.79	0.65
28:2:37:LYS:C	28:2:40:HIS:HE1	2.00	0.65
1:X:1299:A:O2'	1:X:1301:U:OP2	2.14	0.65
1:X:2372:A:H5"	11:I:61:PRO:HA	1.79	0.65
9:G:107:GLN:O	9:G:109:GLY:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:2:ILE:O	10:H:44:TYR:HA	1.96	0.65
10:H:42:LYS:HE3	10:H:44:TYR:O	1.96	0.65
12:J:76:THR:HB	12:J:88:LYS:O	1.96	0.65
13:K:33:ARG:HG3	13:K:114:GLU:HB3	1.77	0.65
1:X:591:G:C2'	1:X:592:G:C8	2.78	0.65
12:J:42:TRP:HB3	12:J:95:VAL:CG1	2.26	0.65
21:S:69:VAL:HG13	21:S:81:VAL:HG22	1.79	0.65
1:X:626:A:C8	5:C:174:GLY:HA3	2.31	0.65
18:P:59:PHE:CD1	26:Z:30:LEU:HD11	2.31	0.65
24:V:2:LYS:HA	24:V:6:MET:HE1	1.78	0.65
1:X:1673:C:H5"	4:B:136:ARG:HB3	1.79	0.65
3:A:87:PRO:O	3:A:88:ASN:HB2	1.97	0.65
5:C:95:LEU:HD21	5:C:99:VAL:HB	1.77	0.65
10:H:42:LYS:NZ	10:H:46:HIS:HD2	1.95	0.65
1:X:227:G:OP2	29:3:8:LYS:HE3	1.95	0.65
1:X:448:C:H5	1:X:449:C:C4	2.14	0.65
1:X:1270:C:H4'	5:C:77:PHE:CE2	2.32	0.65
19:Q:22:ARG:NH1	19:Q:24:VAL:HG21	2.12	0.65
4:B:141:ILE:HG22	4:B:150:VAL:HB	1.79	0.65
5:C:27:LEU:O	5:C:31:VAL:HG22	1.96	0.65
15:M:104:LEU:HD23	15:M:106:TYR:CE2	2.31	0.65
1:X:603:C:H5'	29:3:62:LEU:HD22	1.79	0.65
1:X:617:U:H5	1:X:632:A:N1	1.95	0.65
1:X:2788:C:H2'	1:X:2789:U:H6	1.61	0.65
12:J:77:LYS:O	12:J:79:PRO:HD3	1.97	0.65
14:L:33:ARG:HG2	14:L:38:ILE:HB	1.78	0.65
1:X:177:U:O4	1:X:225:G:C2	2.50	0.65
1:X:2441:U:H2'	1:X:2442:C:C6	2.32	0.65
5:C:176:ASN:HD22	5:C:179:ASP:N	1.89	0.65
1:X:48:A:H4'	1:X:49:U:O5'	1.97	0.64
1:X:754:G:H2'	1:X:755:C:C6	2.31	0.64
15:M:103:LYS:O	15:M:104:LEU:HB2	1.95	0.64
1:X:38:G:C4'	1:X:39:C:OP1	2.44	0.64
7:E:43:VAL:HG23	7:E:52:VAL:HG22	1.79	0.64
1:X:1153:A:OP1	1:X:1153:A:H4'	1.97	0.64
1:X:2328:G:OP2	29:3:42:ARG:HG3	1.97	0.64
16:N:30:LYS:NZ	16:N:30:LYS:HB3	2.13	0.64
1:X:2426:G:C3'	1:X:2479:U:OP2	2.44	0.64
13:K:75:VAL:O	13:K:79:VAL:HG12	1.97	0.64
14:L:31:VAL:HG23	14:L:38:ILE:CD1	2.24	0.64
24:V:37:LEU:HD23	24:V:39:GLN:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2262:C:OP1	27:1:3:LYS:HE2	1.96	0.64
1:X:2426:G:H4'	1:X:2427:A:O5'	1.97	0.64
4:B:49:ILE:HG22	4:B:79:ARG:O	1.97	0.64
6:D:132:ILE:HG13	6:D:154:ILE:HD13	1.79	0.64
17:O:73:LYS:HB2	17:O:82:ARG:HB2	1.78	0.64
18:P:85:MET:CE	18:P:130:GLU:HG3	2.28	0.64
21:S:13:LYS:HB2	21:S:13:LYS:NZ	2.13	0.64
1:X:2265:A:OP1	27:1:28:ARG:HD2	1.97	0.64
1:X:2598:C:C4'	4:B:150:VAL:HG22	2.27	0.64
18:P:41:VAL:HG21	18:P:64:ALA:HB3	1.79	0.64
1:X:26:G:C6	1:X:27:G:N1	2.66	0.64
1:X:163:A:H2'	1:X:164:G:C8	2.33	0.64
1:X:346:C:H2'	1:X:347:C:H6	1.61	0.64
1:X:2660:C:N3	1:X:2707:G:N2	2.46	0.64
1:X:459:A:C2	1:X:466:A:C8	2.86	0.64
1:X:790:A:N7	1:X:806:A:H2	1.95	0.64
1:X:840:U:H4'	1:X:841:G:C2	2.33	0.64
4:B:116:VAL:CG2	4:B:136:ARG:HE	2.05	0.64
11:I:18:ARG:HB2	11:I:21:ARG:HB2	1.80	0.64
19:Q:7:LEU:HD22	19:Q:8:GLN:N	2.12	0.64
26:Z:51:TYR:HA	26:Z:55:ARG:HA	1.78	0.64
1:X:82:G:N2	1:X:83:A:H62	1.96	0.64
1:X:2640:G:H2'	1:X:2641:A:C8	2.33	0.64
3:A:219:LYS:HD2	3:A:219:LYS:O	1.97	0.64
12:J:40:PRO:HB3	12:J:99:LYS:HD2	1.79	0.64
14:L:89:PHE:CZ	14:L:103:LEU:HD22	2.32	0.64
15:M:34:ARG:NH1	15:M:88:VAL:HG21	2.12	0.64
1:X:1182:U:H3	1:X:1193:G:H22	1.45	0.64
12:J:28:VAL:HG21	12:J:135:ARG:HA	1.80	0.64
16:N:99:ALA:HB2	16:N:106:PHE:CE1	2.33	0.64
20:R:85:ASP:HB3	20:R:86:PRO:HD3	1.80	0.64
1:X:1007:A:H1'	17:O:6:GLN:HG2	1.79	0.63
1:X:2533:U:C4	1:X:2534:U:O4	2.51	0.63
2:Y:30:C:OP1	14:L:37:HIS:HB3	1.97	0.63
4:B:49:ILE:HG21	4:B:81:PHE:HE2	1.62	0.63
5:C:95:LEU:CD2	5:C:99:VAL:HB	2.28	0.63
15:M:55:ILE:HB	15:M:103:LYS:O	1.99	0.63
28:2:14:LYS:HA	28:2:14:LYS:HE3	1.80	0.63
1:X:859:U:O2'	1:X:860:U:C2	2.50	0.63
1:X:1329:U:H2'	1:X:1330:G:H8	1.64	0.63
1:X:1685:A:O4'	1:X:1686:A:C2	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1979:C:H4'	1:X:1980:A:OP1	1.97	0.63
1:X:2043:A:O4'	1:X:2481:G:O4'	2.16	0.63
2:Y:51:G:OP1	14:L:97:HIS:HD2	1.81	0.63
19:Q:7:LEU:HD22	19:Q:7:LEU:C	2.18	0.63
4:B:176:ARG:HE	15:M:16:ILE:HG12	1.63	0.63
9:G:132:PHE:HD2	9:G:145:HIS:CG	2.16	0.63
1:X:822:G:C2'	1:X:823:U:H5'	2.29	0.63
1:X:1332:G:C6	1:X:1333:G:O6	2.51	0.63
1:X:1775:A:H4'	1:X:1776:A:O5'	1.98	0.63
3:A:245:ARG:O	3:A:253:LYS:HE2	1.99	0.63
18:P:35:PRO:O	18:P:39:ARG:HD3	1.98	0.63
18:P:126:ILE:HD12	18:P:127:ILE:H	1.63	0.63
1:X:16:G:C2	1:X:535:U:O2	2.51	0.63
1:X:484:G:N1	1:X:485:G:C6	2.66	0.63
1:X:617:U:H5	1:X:632:A:C2	2.16	0.63
1:X:2240:C:C2'	1:X:2241:U:H5'	2.28	0.63
21:S:3:LEU:HD23	21:S:56:VAL:HG22	1.81	0.63
23:U:22:GLY:HA3	23:U:39:LYS:HE3	1.81	0.63
1:X:1392:U:H6	1:X:1392:U:OP1	1.82	0.63
1:X:1469:U:OP1	1:X:1470:G:OP2	2.17	0.63
1:X:1715:A:C8	1:X:1717:A:O4'	2.52	0.63
1:X:2516:U:H2'	1:X:2517:C:C6	2.34	0.63
9:G:154:GLU:O	9:G:157:PRO:HD2	1.98	0.63
12:J:128:ILE:O	12:J:128:ILE:HD12	1.99	0.63
14:L:38:ILE:HD12	14:L:39:TYR:N	2.14	0.63
1:X:458:G:H4'	1:X:459:A:H5'	1.80	0.63
1:X:789:G:O2'	1:X:790:A:OP2	2.11	0.63
4:B:136:ARG:HG2	4:B:137:ARG:N	2.14	0.63
2:Y:17:A:H1'	2:Y:112:A:N9	2.13	0.63
9:G:85:ALA:HB1	9:G:127:ILE:HD13	1.81	0.63
1:X:787:A:H5"	3:A:49:ARG:HH22	1.63	0.62
1:X:968:C:N4	1:X:970:A:C6	2.67	0.62
1:X:2424:G:O2'	1:X:2425:G:H5'	1.99	0.62
5:C:176:ASN:ND2	5:C:179:ASP:H	1.91	0.62
7:E:127:GLU:HG3	7:E:128:PRO:HD2	1.79	0.62
13:K:73:LYS:O	13:K:76:VAL:HG12	1.98	0.62
21:S:168:VAL:HG12	21:S:169:VAL:HG13	1.80	0.62
1:X:1166:A:H5"	16:N:55:ARG:HH11	1.63	0.62
1:X:1827:G:H1'	1:X:1914:U:C2	2.34	0.62
1:X:1856:U:OP1	1:X:2389:G:O2'	2.17	0.62
10:H:47:VAL:HA	10:H:74:VAL:CG1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:81:ASP:O	13:K:85:PRO:HG2	1.98	0.62
15:M:37:THR:HG22	15:M:39:VAL:HG13	1.80	0.62
28:2:25:LYS:HE2	28:2:25:LYS:N	2.14	0.62
1:X:1432:G:O6	1:X:1594:U:H5"	2.00	0.62
1:X:2039:G:H2'	1:X:2039:G:N3	2.14	0.62
1:X:2378:G:H1	1:X:2396:C:H42	1.45	0.62
10:H:109:ARG:HA	10:H:129:LEU:HD13	1.79	0.62
27:1:34:LYS:HE2	27:1:53:LYS:NZ	2.14	0.62
1:X:931:G:H4'	2:Y:83:C:H4'	1.80	0.62
1:X:1837:G:H2'	1:X:1838:G:C8	2.35	0.62
1:X:1919:A:N7	1:X:1928:G:C6	2.67	0.62
1:X:2336:G:N2	1:X:2339:A:OP2	2.32	0.62
1:X:2642:G:H2'	1:X:2643:G:O4'	1.99	0.62
3:A:68:PHE:HE2	3:A:107:LEU:HD11	1.63	0.62
10:H:125:LYS:O	10:H:128:SER:HB2	1.98	0.62
17:O:67:LYS:HD2	17:O:68:LYS:H	1.65	0.62
1:X:1223:G:H5'	1:X:1224:A:H3'	1.81	0.62
1:X:1420:A:C2	1:X:1612:U:O2	2.52	0.62
1:X:1779:C:H2'	1:X:1780:A:C8	2.34	0.62
3:A:211:GLY:HA2	3:A:214:ARG:HG2	1.80	0.62
1:X:685:U:C2	1:X:822:G:N2	2.68	0.62
1:X:2379:G:H1	1:X:2395:C:H42	1.46	0.62
1:X:2705:A:N7	1:X:2707:G:C4	2.68	0.62
13:K:62:SER:O	13:K:66:VAL:HG23	2.00	0.62
16:N:32:TYR:O	16:N:35:ALA:HB3	1.99	0.62
22:T:23:VAL:HA	22:T:38:VAL:HG13	1.82	0.62
1:X:919:U:H2'	1:X:920:G:C8	2.34	0.62
1:X:2011:U:H2'	1:X:2012:A:H8	1.65	0.62
1:X:2518:C:H4'	30:4:3:VAL:HG21	1.82	0.62
1:X:2824:C:H4'	1:X:2825:A:O5'	2.00	0.62
7:E:124:ALA:HB3	7:E:132:ASP:HB3	1.82	0.62
1:X:572:G:H5'	1:X:581:A:H4'	1.81	0.62
1:X:1837:G:H2'	1:X:1838:G:H8	1.64	0.62
4:B:144:ARG:HG2	4:B:145:LYS:N	2.15	0.62
1:X:100:G:H4'	1:X:101:A:OP1	2.00	0.62
1:X:467:U:O2'	1:X:468:A:O5'	2.17	0.62
1:X:1978:U:H2'	1:X:1979:C:C6	2.35	0.62
12:J:40:PRO:HB3	12:J:99:LYS:CD	2.30	0.62
1:X:75:C:O2	1:X:109:A:H2	1.83	0.62
1:X:1811:A:H1'	1:X:1812:U:OP2	2.00	0.62
4:B:147:PRO:O	4:B:149:ARG:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:72:ASP:CG	13:K:75:VAL:HG23	2.20	0.62
20:R:15:HIS:ND1	20:R:16:PHE:CD2	2.63	0.62
20:R:16:PHE:HZ	20:R:46:VAL:HG22	1.65	0.62
1:X:334:G:H4'	1:X:335:A:O5'	1.98	0.61
1:X:757:U:O2'	1:X:758:G:H5'	2.00	0.61
1:X:2426:G:C4	1:X:2479:U:H5	2.18	0.61
5:C:128:ALA:O	5:C:130:THR:N	2.31	0.61
10:H:42:LYS:HZ2	10:H:46:HIS:HD2	1.47	0.61
12:J:92:GLU:HG3	12:J:93:TYR:HD2	1.65	0.61
15:M:104:LEU:HA	15:M:106:TYR:HE2	1.64	0.61
1:X:663:G:H3'	1:X:664:C:H5"	1.81	0.61
9:G:104:THR:OG1	9:G:105:GLY:N	2.32	0.61
10:H:116:ARG:HD2	15:M:38:LYS:HZ1	1.65	0.61
18:P:14:ARG:HA	18:P:17:GLN:HG2	1.82	0.61
1:X:334:G:C2'	5:C:162:ARG:HD3	2.29	0.61
1:X:2011:U:H2'	1:X:2012:A:C8	2.34	0.61
1:X:2598:C:O4'	4:B:150:VAL:HG22	1.99	0.61
11:I:56:LEU:HD22	29:3:52:LYS:HZ2	1.65	0.61
29:3:34:THR:OG1	29:3:41:ILE:HD11	1.99	0.61
1:X:2026:C:N4	1:X:2757:G:C2	2.69	0.61
14:L:89:PHE:HB3	14:L:91:ARG:HH21	1.64	0.61
19:Q:12:ILE:O	19:Q:12:ILE:HG12	1.99	0.61
1:X:218:A:C8	1:X:220:U:C2	2.88	0.61
1:X:1164:C:H2'	1:X:1165:G:O4'	2.01	0.61
1:X:1479:G:H2'	1:X:1480:G:C8	2.35	0.61
8:F:112:MET:HB2	8:F:113:PRO:HD3	1.80	0.61
11:I:56:LEU:HB3	29:3:52:LYS:HE3	1.82	0.61
28:2:10:ARG:H	28:2:10:ARG:CD	1.97	0.61
1:X:1225:G:H2'	1:X:1249:G:H22	1.65	0.61
1:X:2409:A:C4'	1:X:2410:U:OP1	2.48	0.61
1:X:2604:G:H2'	1:X:2605:C:C6	2.36	0.61
5:C:102:LEU:O	5:C:102:LEU:HD23	2.00	0.61
15:M:28:ARG:HB2	15:M:29:PRO:CD	2.19	0.61
1:X:736:G:H2'	1:X:737:C:O4'	2.01	0.61
1:X:2064:U:H5"	23:U:43:ARG:HH11	1.66	0.61
1:X:2690:A:OP1	1:X:2692:A:P	2.58	0.61
21:S:127:PRO:O	21:S:128:ARG:HG2	2.00	0.61
27:1:28:ARG:HB2	27:1:30:ASN:OD1	2.01	0.61
1:X:1096:A:C4'	1:X:1097:A:OP1	2.47	0.61
1:X:1964:A:H5"	1:X:1965:U:OP2	1.99	0.61
14:L:33:ARG:HE	14:L:38:ILE:HB	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:92:VAL:HG13	18:P:126:ILE:CD1	2.29	0.61
19:Q:35:LYS:HD3	19:Q:53:ILE:HG23	1.82	0.61
24:V:25:LEU:HD13	24:V:46:LEU:HD12	1.82	0.61
1:X:38:G:H1'	1:X:39:C:O5'	2.01	0.61
1:X:163:A:H2'	1:X:164:G:H8	1.66	0.61
1:X:971:A:N6	12:J:83:ARG:HH22	1.99	0.61
1:X:2064:U:H5"	23:U:43:ARG:NH1	2.16	0.61
9:G:55:ALA:C	9:G:134:MET:HE1	2.20	0.61
11:I:51:GLY:O	11:I:55:ARG:NH1	2.31	0.61
25:W:23:LEU:HD21	25:W:43:MET:HB3	1.82	0.61
1:X:529:U:H2'	1:X:530:G:H8	1.66	0.61
1:X:2310:G:H4'	22:T:43:THR:H	1.66	0.61
9:G:89:ALA:C	9:G:90:LEU:HD12	2.22	0.61
11:I:62:LYS:HG2	11:I:63:ARG:H	1.66	0.61
11:I:107:LYS:HG2	11:I:109:LEU:HD21	1.83	0.61
1:X:688:A:H62	1:X:816:U:H3	1.49	0.60
1:X:1438:G:C2'	1:X:1439:G:H5'	2.31	0.60
1:X:2222:U:H2'	1:X:2223:U:C6	2.36	0.60
2:Y:9:G:H5"	14:L:32:TYR:CD1	2.36	0.60
21:S:49:THR:OG1	21:S:132:GLN:HA	2.00	0.60
1:X:538:A:O2'	1:X:539:A:H5"	2.01	0.60
1:X:613:A:C6	1:X:668:A:H1'	2.37	0.60
1:X:638:A:C8	11:I:74:VAL:HG11	2.36	0.60
1:X:692:C:H42	1:X:811:G:H1	1.49	0.60
1:X:2201:G:H5'	3:A:189:GLU:OE1	2.00	0.60
12:J:64:LYS:HZ3	12:J:110:VAL:HG13	1.66	0.60
13:K:24:GLN:HB3	13:K:44:LEU:HD22	1.83	0.60
15:M:39:VAL:HG12	15:M:45:THR:CG2	2.31	0.60
27:1:34:LYS:HE2	27:1:53:LYS:HZ2	1.66	0.60
1:X:178:C:O5'	23:U:40:ARG:NH2	2.33	0.60
1:X:1288:A:H2	1:X:1662:G:H21	1.47	0.60
1:X:2662:C:O2	10:H:82:LYS:NZ	2.33	0.60
1:X:2859:U:N3	26:Z:52:TYR:CE1	2.69	0.60
3:A:71:ARG:HH12	3:A:150:PRO:HB3	1.66	0.60
11:I:29:THR:O	11:I:30:ALA:HB3	2.01	0.60
15:M:5:ILE:HD13	15:M:7:ILE:HG22	1.81	0.60
16:N:22:LYS:HG3	16:N:23:GLY:H	1.66	0.60
1:X:192:G:H4'	1:X:193:A:H4'	1.83	0.60
1:X:753:U:H2'	1:X:754:G:C8	2.37	0.60
1:X:935:C:H1'	22:T:29:GLU:HG2	1.81	0.60
1:X:999:A:H5"	25:W:8:SER:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1357:U:O2'	1:X:1358:C:P	2.59	0.60
1:X:2016:A:O2'	1:X:2018:G:OP2	2.18	0.60
1:X:2048:C:H1'	1:X:2428:U:N3	2.17	0.60
2:Y:33:C:N4	2:Y:53:G:H1	1.97	0.60
3:A:49:ARG:HD2	3:A:49:ARG:N	2.10	0.60
5:C:15:ILE:HD11	5:C:195:ILE:H	1.67	0.60
11:I:91:ASP:HA	11:I:94:GLU:OE2	2.01	0.60
28:2:17:GLY:O	28:2:20:ALA:HB3	2.01	0.60
1:X:1744:G:N2	1:X:1747:G:OP2	2.31	0.60
31:X:2881:LMA:O55	31:X:2881:LMA:H12	2.00	0.60
4:B:134:TRP:O	4:B:135:HIS:C	2.40	0.60
4:B:155:ARG:HG3	4:B:155:ARG:NH1	2.15	0.60
7:E:87:LEU:HB2	7:E:131:ILE:HB	1.82	0.60
7:E:154:PRO:HA	7:E:160:LYS:O	2.01	0.60
15:M:34:ARG:NH1	15:M:81:PHE:HB3	2.15	0.60
29:3:31:HIS:O	29:3:32:GLN:C	2.39	0.60
1:X:455:A:H2	1:X:1258:G:N3	1.99	0.60
1:X:521:U:H5"	1:X:522:G:OP2	2.01	0.60
1:X:817:A:H5"	1:X:818:G:OP1	2.01	0.60
1:X:1226:A:C8	1:X:1250:A:H2	2.18	0.60
1:X:2311:U:H4'	1:X:2315:A:N6	2.16	0.60
5:C:151:VAL:CG1	5:C:173:ALA:HA	2.31	0.60
12:J:29:ALA:HB3	12:J:68:ARG:HH21	1.65	0.60
28:2:15:THR:O	28:2:16:HIS:HB2	2.02	0.60
1:X:695:G:H5"	28:2:26:SER:HB2	1.83	0.60
1:X:1666:G:H1	1:X:1991:C:H42	1.47	0.60
1:X:2229:G:H5'	12:J:84:MET:HG2	1.83	0.60
1:X:2782:G:H2'	1:X:2783:U:O5'	2.01	0.60
1:X:2796:A:H2'	1:X:2797:G:H8	1.66	0.60
13:K:73:LYS:HA	13:K:76:VAL:HG12	1.83	0.60
16:N:62:ILE:HG23	16:N:76:TYR:CE1	2.37	0.60
17:O:36:LYS:NZ	17:O:54:TYR:HB3	2.15	0.60
1:X:28:A:H1'	1:X:523:A:C2	2.37	0.60
1:X:48:A:H4'	1:X:49:U:C5'	2.32	0.60
1:X:1479:G:H2'	1:X:1480:G:H8	1.67	0.60
1:X:1693:A:N3	1:X:1976:U:H5'	2.16	0.60
1:X:1770:U:H5	1:X:1775:A:N7	2.00	0.60
1:X:1977:C:H2'	1:X:1977:C:O2	2.02	0.60
1:X:2616:U:H5"	4:B:82:ARG:NH2	2.16	0.60
6:D:5:LYS:O	6:D:8:TYR:HB3	2.01	0.60
6:D:60:ILE:HG22	6:D:140:GLU:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:94:PHE:HE2	7:E:160:LYS:HB3	1.66	0.60
10:H:16:ALA:HB3	10:H:98:ILE:HD11	1.82	0.60
16:N:25:TRP:CE3	16:N:26:GLY:CA	2.85	0.60
1:X:1886:G:O2'	1:X:1887:G:H5'	2.02	0.60
1:X:2074:U:H3'	1:X:2075:U:H5"	1.83	0.60
1:X:2700:U:O2	1:X:2700:U:H2'	2.02	0.60
21:S:155:PRO:HG2	21:S:158:CYS:SG	2.42	0.60
22:T:47:ALA:HB1	22:T:51:VAL:O	2.02	0.60
1:X:760:U:C5	26:Z:3:LYS:HG3	2.37	0.59
1:X:1016:C:O2'	1:X:1023:U:C5	2.54	0.59
1:X:1050:G:H1	1:X:1127:C:H42	1.49	0.59
1:X:1399:C:H2'	1:X:1400:A:H8	1.66	0.59
1:X:1468:A:OP2	1:X:1468:A:H8	1.85	0.59
19:Q:68:PHE:O	19:Q:69:ILE:HD12	2.01	0.59
26:Z:10:LYS:HG2	26:Z:11:THR:N	2.15	0.59
1:X:122:G:H2'	28:2:19:ARG:HH21	1.67	0.59
1:X:1329:U:O2'	1:X:1330:G:H5'	2.02	0.59
1:X:1337:G:C2	1:X:1341:G:N1	2.70	0.59
1:X:1505:U:H2'	1:X:1506:C:H5"	1.85	0.59
1:X:1751:A:H2'	1:X:1752:U:C6	2.37	0.59
1:X:2736:U:H5"	30:4:19:ARG:CG	2.32	0.59
5:C:176:ASN:HB3	5:C:179:ASP:OD2	2.02	0.59
16:N:79:PHE:HE2	16:N:95:LEU:HD21	1.66	0.59
19:Q:31:PRO:HA	19:Q:76:LYS:HD2	1.82	0.59
1:X:314:G:N1	1:X:326:A:C2	2.71	0.59
1:X:538:A:H4'	1:X:539:A:OP1	2.02	0.59
1:X:699:G:C6	28:2:12:ARG:HA	2.37	0.59
1:X:1925:C:H2'	1:X:1926:U:C5	2.37	0.59
5:C:27:LEU:HD23	5:C:181:LEU:HD22	1.84	0.59
9:G:61:ARG:HG2	9:G:65:LYS:HD2	1.82	0.59
18:P:39:ARG:HD2	18:P:97:VAL:HB	1.84	0.59
18:P:92:VAL:HG13	18:P:126:ILE:HD11	1.83	0.59
18:P:106:LEU:HD23	18:P:106:LEU:C	2.23	0.59
1:X:761:G:OP2	18:P:110:ALA:CB	2.50	0.59
1:X:1314:A:H2	1:X:1642:G:H21	1.50	0.59
1:X:1433:A:H62	1:X:1435:G:H1'	1.67	0.59
10:H:29:ILE:HG21	10:H:123:PHE:CE1	2.37	0.59
17:O:19:VAL:HG13	17:O:90:PHE:CD1	2.37	0.59
20:R:38:LEU:HB2	20:R:47:VAL:CG2	2.33	0.59
28:2:34:ARG:HH11	28:2:42:LEU:HG	1.67	0.59
1:X:824:U:O2'	11:I:30:ALA:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1182:U:C4'	1:X:1183:C:OP1	2.50	0.59
1:X:1623:C:H4'	1:X:1624:A:O5'	2.02	0.59
1:X:2350:G:O2'	27:1:46:LYS:HB3	2.03	0.59
5:C:163:ASN:ND2	5:C:167:VAL:H	1.97	0.59
6:D:13:ARG:HB3	6:D:14:PRO:HD3	1.84	0.59
10:H:13:ASN:ND2	10:H:109:ARG:HG2	2.16	0.59
1:X:1173:G:H2'	1:X:1174:G:H8	1.68	0.59
1:X:1361:G:H1	1:X:1614:C:N4	2.01	0.59
1:X:2245:A:H4'	1:X:2246:A:C2	2.37	0.59
6:D:117:ILE:HD12	6:D:175:LEU:HD11	1.83	0.59
13:K:13:ASN:OD1	13:K:14:SER:N	2.35	0.59
14:L:60:LYS:HZ2	14:L:64:LYS:HE2	1.68	0.59
17:O:15:SER:HA	17:O:95:ILE:O	2.03	0.59
1:X:13:A:N3	1:X:15:G:C6	2.71	0.59
1:X:338:G:H1'	20:R:10:HIS:HE1	1.67	0.59
1:X:597:U:H2'	1:X:598:U:H6	1.67	0.59
1:X:1310:C:H2'	1:X:1311:C:H6	1.66	0.59
1:X:1909:U:H5	1:X:1910:A:H62	1.49	0.59
1:X:2010:G:O6	1:X:2016:A:C8	2.55	0.59
1:X:2845:C:H3'	1:X:2845:C:H6	1.67	0.59
17:O:11:GLN:HE22	17:O:38:LEU:HD12	1.68	0.59
20:R:81:VAL:HG11	20:R:89:GLY:CA	2.32	0.59
1:X:29:U:O5'	1:X:29:U:H6	1.85	0.59
1:X:1976:U:H5"	4:B:128:SER:HB3	1.83	0.59
4:B:14:ILE:HA	15:M:20:HIS:CD2	2.26	0.59
12:J:44:LYS:HD3	12:J:47:GLN:NE2	2.17	0.59
1:X:762:A:H2	1:X:766:A:HO2'	1.48	0.59
10:H:133:VAL:HG12	10:H:133:VAL:O	2.01	0.59
1:X:40:U:H2'	1:X:41:G:O4'	2.02	0.59
1:X:57:G:C4	1:X:69:G:N2	2.71	0.59
1:X:321:A:C2	1:X:323:G:H1'	2.38	0.59
1:X:1234:C:O2	1:X:1242:A:C2	2.56	0.59
1:X:1665:C:H2'	1:X:1666:G:O4'	2.03	0.59
1:X:1996:A:C2	18:P:109:ARG:NH2	2.71	0.59
1:X:2209:G:H5"	23:U:46:LEU:HB2	1.83	0.59
31:X:2881:LMA:H34B	31:X:2881:LMA:C54	2.33	0.59
3:A:25:LEU:CB	3:A:206:VAL:H	2.15	0.59
7:E:7:GLN:O	7:E:9:ILE:HG13	2.02	0.59
20:R:38:LEU:HB2	20:R:47:VAL:HG23	1.83	0.59
24:V:43:VAL:O	24:V:47:ARG:HG2	2.03	0.59
1:X:712:A:H2'	1:X:713:G:O4'	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1430:G:H2'	1:X:1431:U:C6	2.38	0.58
1:X:1684:G:C2	1:X:1974:U:C5	2.91	0.58
10:H:28:GLY:O	10:H:35:THR:OG1	2.11	0.58
1:X:1466:C:C2'	1:X:1467:U:O4'	2.47	0.58
1:X:2781:G:C2'	1:X:2782:G:H5"	2.32	0.58
4:B:116:VAL:HG22	4:B:136:ARG:CD	2.32	0.58
5:C:26:VAL:HG22	11:I:18:ARG:NH1	2.13	0.58
12:J:40:PRO:CB	12:J:99:LYS:HZ2	2.15	0.58
12:J:92:GLU:HG3	12:J:93:TYR:CD2	2.38	0.58
1:X:177:U:H3'	23:U:40:ARG:NH2	2.18	0.58
1:X:1270:C:O2	5:C:78:VAL:HG23	2.02	0.58
1:X:2674:C:O2'	1:X:2675:U:H5'	2.03	0.58
20:R:29:HIS:HD2	20:R:51:VAL:HG22	1.67	0.58
21:S:120:LEU:HD23	21:S:121:GLN:N	2.18	0.58
1:X:1468:A:H8	1:X:1468:A:P	2.26	0.58
9:G:62:ILE:O	9:G:77:GLY:HA3	2.03	0.58
16:N:24:PHE:HB2	16:N:29:SER:HB3	1.86	0.58
1:X:555:U:H3'	1:X:556:A:H8	1.67	0.58
1:X:757:U:C2'	1:X:758:G:H5'	2.33	0.58
1:X:1628:C:H5'	28:2:7:PRO:HG2	1.85	0.58
1:X:1699:A:H61	1:X:1723:U:H3	1.52	0.58
1:X:2256:G:OP2	12:J:86:LYS:HD2	2.04	0.58
1:X:2625:U:O5'	1:X:2625:U:H6	1.84	0.58
16:N:40:LEU:HB3	17:O:74:TYR:CE2	2.38	0.58
1:X:306:G:N2	1:X:355:G:H1'	2.19	0.58
1:X:334:G:H2'	5:C:162:ARG:HD3	1.86	0.58
1:X:540:G:C2'	1:X:542:A:C2	2.84	0.58
1:X:547:U:H1'	9:G:73:ASN:HD21	1.68	0.58
1:X:1433:A:C4	1:X:1595:A:H2	2.21	0.58
1:X:923:A:C5	12:J:12:LYS:HE2	2.39	0.58
1:X:1304:U:O2'	1:X:1305:C:H5'	2.04	0.58
1:X:2323:U:O2'	27:1:38:LYS:HB3	2.04	0.58
1:X:2796:A:H2'	1:X:2797:G:C8	2.39	0.58
4:B:59:VAL:HG21	4:B:74:PRO:HB3	1.85	0.58
7:E:90:ARG:HH21	7:E:163:ARG:NH1	2.01	0.58
29:3:8:LYS:HG3	29:3:12:ARG:NH1	2.17	0.58
1:X:2695:C:H2'	1:X:2696:A:H8	1.69	0.58
3:A:131:ALA:HA	3:A:192:ALA:O	2.03	0.58
19:Q:35:LYS:HA	19:Q:38:ILE:CG2	2.32	0.58
1:X:721:C:H42	1:X:736:G:H1	1.52	0.58
1:X:836:G:H2'	1:X:837:U:H6	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1919:A:H1'	1:X:1923:U:N3	2.18	0.58
1:X:2237:C:H3'	1:X:2238:G:H5'	1.86	0.58
4:B:118:LYS:HG2	4:B:160:MET:SD	2.43	0.58
27:1:14:SER:HB2	27:1:23:THR:H	1.67	0.58
1:X:797:A:N7	3:A:230:VAL:HG21	2.18	0.58
1:X:839:U:H5"	1:X:2408:G:P	2.44	0.58
1:X:2339:A:OP1	29:3:49:VAL:HG22	2.04	0.58
5:C:62:LYS:HD3	5:C:63:GLY:N	2.19	0.58
19:Q:61:LYS:HB2	19:Q:72:ARG:HD3	1.86	0.58
22:T:12:ASN:CB	22:T:14:ARG:HG2	2.29	0.58
23:U:78:ILE:HD13	23:U:79:GLU:N	2.19	0.58
26:Z:51:TYR:CD2	26:Z:55:ARG:HB2	2.39	0.58
1:X:1496:G:C4'	1:X:1497:C:OP1	2.52	0.57
17:O:5:ILE:HD11	17:O:9:GLY:HA2	1.84	0.57
1:X:820:U:OP1	11:I:40:ARG:NH2	2.37	0.57
1:X:1469:U:C5'	1:X:1470:G:OP2	2.51	0.57
1:X:2522:G:C6	1:X:2523:G:C6	2.92	0.57
3:A:207:LEU:HA	3:A:212:ARG:HH11	1.69	0.57
17:O:68:LYS:HD2	17:O:69:ILE:N	2.19	0.57
27:1:40:TYR:HB2	27:1:50:PHE:CD2	2.38	0.57
28:2:42:LEU:N	28:2:42:LEU:CD1	2.66	0.57
1:X:318:G:H21	1:X:341:A:H62	1.53	0.57
1:X:761:G:OP2	18:P:110:ALA:HB2	2.04	0.57
1:X:1674:C:H2'	1:X:1675:C:C6	2.40	0.57
1:X:2447:G:O2'	1:X:2448:A:C8	2.51	0.57
1:X:2663:U:C4	1:X:2664:G:N7	2.72	0.57
3:A:109:PRO:HA	3:A:197:VAL:HA	1.86	0.57
4:B:100:GLU:O	4:B:172:VAL:HG23	2.03	0.57
7:E:16:THR:HB	7:E:27:LYS:HB2	1.85	0.57
18:P:37:LYS:O	18:P:40:LEU:HB2	2.04	0.57
1:X:577:U:H2'	1:X:579:G:OP2	2.03	0.57
1:X:760:U:C6	26:Z:3:LYS:CE	2.81	0.57
1:X:1142:G:N3	9:G:103:TYR:CD2	2.68	0.57
1:X:1182:U:H4'	1:X:1183:C:OP1	2.04	0.57
27:1:8:ILE:O	27:1:9:ILE:HG12	2.04	0.57
1:X:684:C:H5	11:I:43:ALA:HA	1.69	0.57
1:X:1224:A:H5'	18:P:10:ASN:ND2	2.19	0.57
1:X:1850:G:H21	1:X:1867:A:H8	1.50	0.57
3:A:43:GLY:C	3:A:44:ARG:NH1	2.55	0.57
3:A:244:GLY:H	3:A:245:ARG:HH11	1.45	0.57
15:M:67:THR:OG1	15:M:80:VAL:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:555:U:H3'	1:X:556:A:C8	2.39	0.57
1:X:637:G:H1	11:I:101:ARG:HD3	1.70	0.57
1:X:759:C:C2'	1:X:760:U:OP2	2.52	0.57
1:X:923:A:H5"	1:X:924:C:C5'	2.34	0.57
1:X:2617:G:HO2'	1:X:2618:A:H8	1.51	0.57
6:D:13:ARG:HG3	6:D:28:VAL:HG21	1.86	0.57
10:H:1:MET:N	10:H:1:MET:HE2	2.20	0.57
20:R:20:ASP:O	20:R:36:VAL:HG23	2.05	0.57
1:X:487:G:H4'	1:X:512:A:N1	2.20	0.57
1:X:1441:A:O4'	1:X:1442:C:C6	2.58	0.57
1:X:2571:G:C6	1:X:2572:U:C2	2.92	0.57
4:B:136:ARG:CG	4:B:137:ARG:H	2.18	0.57
9:G:70:PHE:HB2	16:N:64:ARG:NE	2.19	0.57
12:J:22:ALA:HB2	12:J:100:PRO:O	2.05	0.57
22:T:43:THR:HG23	22:T:46:LYS:HG2	1.86	0.57
1:X:567:G:H5'	9:G:140:GLN:OE1	2.04	0.57
1:X:750:C:C4	1:X:751:G:N7	2.73	0.57
5:C:148:VAL:HG22	5:C:185:ARG:HB2	1.86	0.57
7:E:117:PRO:HD3	7:E:123:PHE:HE1	1.70	0.57
9:G:61:ARG:HE	9:G:65:LYS:CD	2.17	0.57
15:M:50:PHE:CZ	15:M:70:LYS:HB3	2.39	0.57
23:U:17:SER:CB	23:U:44:ALA:HA	2.25	0.57
1:X:173:A:H2'	1:X:173:A:N3	2.18	0.57
1:X:538:A:N6	1:X:2026:C:O5'	2.37	0.57
1:X:623:G:H21	1:X:626:A:H2	1.53	0.57
1:X:1223:G:H4'	1:X:1224:A:O5'	2.05	0.57
1:X:1773:C:O2'	1:X:2588:U:H5"	2.05	0.57
1:X:1918:G:C4	1:X:1945:C:N4	2.73	0.57
1:X:1967:U:H2'	1:X:1968:G:H8	1.68	0.57
1:X:2262:C:H5'	27:1:7:ARG:HH22	1.70	0.57
1:X:2490:U:H2'	1:X:2491:C:O4'	2.05	0.57
4:B:136:ARG:HG2	4:B:137:ARG:H	1.68	0.57
9:G:75:ILE:HG13	9:G:75:ILE:O	2.04	0.57
10:H:85:ASP:OD2	10:H:87:SER:N	2.37	0.57
11:I:56:LEU:HB3	29:3:52:LYS:CE	2.34	0.57
13:K:18:VAL:HG12	13:K:19:ALA:N	2.20	0.57
13:K:51:LEU:CD2	13:K:70:ILE:HD11	2.34	0.57
1:X:88:G:C8	1:X:89:A:C8	2.92	0.57
1:X:836:G:H2'	1:X:837:U:C6	2.39	0.57
1:X:2494:C:O2'	1:X:2495:G:H5'	2.04	0.57
1:X:2545:A:H61	10:H:40:GLY:HA3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2671:C:O2'	1:X:2672:U:H5'	2.05	0.57
19:Q:62:ARG:NH1	19:Q:73:ASN:ND2	2.52	0.57
1:X:494:A:H5'	20:R:58:VAL:HG22	1.87	0.56
1:X:1135:C:H2'	1:X:1136:G:O4'	2.03	0.56
1:X:1322:G:H4'	28:2:7:PRO:HB2	1.87	0.56
1:X:1696:C:C5	1:X:1697:U:C5	2.93	0.56
1:X:2728:A:O2'	7:E:63:ALA:HA	2.04	0.56
31:X:2881:LMA:O53	31:X:2881:LMA:C32	2.50	0.56
7:E:15:VAL:HG11	7:E:76:VAL:HG13	1.87	0.56
15:M:34:ARG:HD3	15:M:88:VAL:HG22	1.87	0.56
1:X:617:U:C5	1:X:632:A:N1	2.74	0.56
1:X:1644:G:O2'	1:X:1645:U:H5'	2.05	0.56
1:X:2426:G:H1'	1:X:2427:A:OP2	2.05	0.56
1:X:2757:G:C5'	1:X:2758:A:H5'	2.31	0.56
11:I:89:ASP:OD2	11:I:120:VAL:HA	2.05	0.56
1:X:503:G:H2'	1:X:504:G:O4'	2.05	0.56
1:X:686:C:C2'	1:X:687:G:H5'	2.35	0.56
1:X:825:C:H5'	11:I:30:ALA:HB1	1.86	0.56
1:X:1033:G:H2'	9:G:97:ASP:OD1	2.04	0.56
1:X:1687:C:H4'	1:X:1977:C:O2'	2.06	0.56
1:X:1769:U:C5	1:X:1775:A:C2	2.94	0.56
1:X:2372:A:H5"	11:I:61:PRO:CA	2.35	0.56
1:X:2728:A:C2	1:X:2737:A:C5	2.93	0.56
2:Y:25:G:H2'	2:Y:26:G:C5	2.40	0.56
4:B:34:VAL:HG21	4:B:78:LEU:HD22	1.88	0.56
6:D:108:LEU:HB2	6:D:109:PRO:HD3	1.87	0.56
9:G:141:GLY:O	9:G:144:MET:N	2.37	0.56
23:U:52:ARG:HG3	23:U:62:LEU:HD22	1.85	0.56
26:Z:58:LEU:HD12	26:Z:58:LEU:N	2.20	0.56
28:2:34:ARG:HH11	28:2:42:LEU:HA	1.70	0.56
1:X:48:A:N6	1:X:154:U:H5	2.04	0.56
1:X:459:A:H4'	1:X:461:A:C8	2.40	0.56
1:X:540:G:H5"	1:X:541:C:OP2	2.05	0.56
1:X:1016:C:O2'	1:X:1023:U:H5	1.86	0.56
1:X:1949:A:N6	1:X:2581:A:H62	2.03	0.56
1:X:2634:G:O2'	1:X:2635:U:C5	2.59	0.56
1:X:2845:C:H3'	1:X:2845:C:C6	2.40	0.56
5:C:102:LEU:HD21	5:C:106:MET:CE	2.35	0.56
13:K:90:ARG:HG3	13:K:90:ARG:O	2.05	0.56
24:V:25:LEU:HD13	24:V:46:LEU:HB2	1.87	0.56
1:X:219:G:H2'	1:X:220:U:OP2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1006:C:OP2	16:N:54:LYS:NZ	2.23	0.56
1:X:1073:G:H21	8:F:133:SER:HB3	1.69	0.56
2:Y:107:C:H2'	2:Y:108:G:O4'	2.06	0.56
7:E:57:ASP:HB3	7:E:62:ARG:HH11	1.70	0.56
15:M:39:VAL:CG1	15:M:45:THR:HG23	2.35	0.56
19:Q:11:VAL:HG23	19:Q:27:PHE:HA	1.87	0.56
22:T:51:VAL:HG21	22:T:79:ILE:O	2.06	0.56
1:X:88:G:H3'	1:X:89:A:H5"	1.88	0.56
1:X:1016:C:H1'	1:X:1023:U:C5	2.41	0.56
1:X:1129:A:C6	1:X:1130:U:N3	2.74	0.56
1:X:1218:C:H4'	11:I:13:ARG:HH11	1.69	0.56
1:X:2262:C:H2'	1:X:2263:C:O4'	2.05	0.56
1:X:2383:C:H2'	1:X:2384:G:O4'	2.05	0.56
4:B:7:THR:CG2	4:B:193:GLY:HA2	2.35	0.56
10:H:132:GLU:HB2	15:M:73:PHE:HE1	1.71	0.56
13:K:76:VAL:O	13:K:80:MET:HB2	2.05	0.56
17:O:78:VAL:O	17:O:79:GLN:HB2	2.06	0.56
1:X:1478:U:H2'	1:X:1479:G:H8	1.70	0.56
1:X:1712:G:H2'	1:X:1713:G:H5'	1.88	0.56
1:X:2016:A:C5	1:X:2019:C:C4	2.94	0.56
4:B:56:GLU:HG2	4:B:74:PRO:HG2	1.87	0.56
5:C:187:VAL:O	5:C:187:VAL:HG12	2.05	0.56
11:I:85:ASP:HA	11:I:116:ARG:HH12	1.71	0.56
20:R:25:LEU:HD23	20:R:26:SER:HB3	1.87	0.56
24:V:25:LEU:CD1	24:V:46:LEU:HD12	2.36	0.56
1:X:760:U:HO2'	1:X:761:G:P	2.28	0.56
1:X:877:G:H1	1:X:924:C:H42	1.54	0.56
1:X:1834:G:N2	1:X:1884:A:C6	2.73	0.56
1:X:1967:U:H2'	1:X:1968:G:C8	2.40	0.56
1:X:2073:A:H61	1:X:2208:U:H3	1.52	0.56
1:X:2170:C:H3'	1:X:2171:U:C5'	2.32	0.56
1:X:2844:G:C2	1:X:2845:C:O2	2.58	0.56
26:Z:31:THR:HG22	26:Z:32:GLU:N	2.21	0.56
1:X:101:A:H2'	1:X:102:C:O4'	2.06	0.56
1:X:305:A:C2	1:X:356:A:C2	2.94	0.56
1:X:1068:A:H2'	1:X:1069:G:C8	2.41	0.56
1:X:1310:C:H2'	1:X:1311:C:C6	2.41	0.56
1:X:1407:G:H4'	1:X:1619:A:H4'	1.87	0.56
1:X:1423:A:C2	1:X:1609:G:C2	2.94	0.56
1:X:2323:U:H3'	27:1:39:LYS:O	2.05	0.56
1:X:2734:U:H4'	30:4:26:ILE:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:90:C:H2'	2:Y:91:A:O4'	2.06	0.56
7:E:7:GLN:HB2	7:E:8:PRO:HD3	1.88	0.56
10:H:75:VAL:HG12	10:H:118:LEU:CD2	2.36	0.56
12:J:42:TRP:CB	12:J:95:VAL:HG11	2.31	0.56
14:L:37:HIS:NE2	14:L:39:TYR:CZ	2.74	0.56
1:X:1310:C:C2	1:X:1311:C:C5	2.94	0.56
1:X:1810:U:OP2	3:A:158:ARG:HD3	2.06	0.56
1:X:2499:C:C2'	1:X:2500:C:H5'	2.35	0.56
1:X:2666:U:O2'	1:X:2667:C:H5'	2.06	0.56
4:B:85:ALA:N	4:B:86:PRO:HD3	2.21	0.56
1:X:177:U:C4'	23:U:40:ARG:HE	2.19	0.55
1:X:2397:A:H2'	1:X:2398:U:O4'	2.06	0.55
3:A:159:SER:O	3:A:197:VAL:HG21	2.06	0.55
6:D:118:ASN:HB3	6:D:122:PHE:HZ	1.69	0.55
12:J:32:ASP:H	12:J:108:ALA:HB2	1.70	0.55
17:O:13:ARG:HD2	17:O:95:ILE:HG13	1.88	0.55
19:Q:20:MET:HA	19:Q:24:VAL:O	2.06	0.55
25:W:4:LYS:CG	25:W:52:GLU:HB3	2.36	0.55
26:Z:14:SER:O	26:Z:18:MET:HG3	2.06	0.55
27:1:14:SER:HB3	27:1:50:PHE:CZ	2.41	0.55
1:X:393:U:H1'	23:U:18:VAL:HG21	1.88	0.55
1:X:516:G:H4'	1:X:519:C:O2	2.07	0.55
1:X:538:A:H5"	9:G:142:ARG:HH12	1.72	0.55
1:X:1329:U:H2'	1:X:1330:G:C8	2.41	0.55
1:X:2672:U:H2'	1:X:2673:G:C8	2.38	0.55
2:Y:58:G:H4'	2:Y:59:A:H8	1.70	0.55
14:L:38:ILE:HD11	14:L:40:ALA:N	2.21	0.55
21:S:51:LEU:H	21:S:51:LEU:CD2	2.18	0.55
1:X:521:U:O4	1:X:522:G:N2	2.40	0.55
1:X:967:G:O6	12:J:17:ARG:NH2	2.38	0.55
1:X:1333:G:C2	1:X:1342:U:H5'	2.41	0.55
1:X:1466:C:C5	1:X:1467:U:O2	2.59	0.55
1:X:1643:A:H61	1:X:1656:U:H3	1.54	0.55
10:H:80:ALA:HB2	10:H:90:ARG:HD3	1.87	0.55
16:N:93:LYS:O	16:N:94:VAL:HB	2.06	0.55
26:Z:31:THR:O	26:Z:39:LYS:HA	2.06	0.55
1:X:496:C:C2'	1:X:497:C:H5'	2.35	0.55
1:X:760:U:C5	26:Z:3:LYS:HE2	2.41	0.55
1:X:807:A:H2'	1:X:808:C:H6	1.71	0.55
1:X:969:U:O4	12:J:18:MET:HA	2.06	0.55
1:X:2426:G:C4	1:X:2479:U:C5	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:26:VAL:O	5:C:30:VAL:HG23	2.06	0.55
15:M:102:ALA:O	15:M:103:LYS:HD2	2.06	0.55
1:X:70:A:OP2	1:X:111:G:H4'	2.06	0.55
1:X:1299:A:HO2'	1:X:1301:U:P	2.29	0.55
1:X:1474:A:H2'	1:X:1474:A:N3	2.22	0.55
1:X:1684:G:N3	1:X:1974:U:C5	2.75	0.55
1:X:2251:U:H5"	1:X:2252:A:OP1	2.06	0.55
1:X:2274:C:OP2	14:L:11:LEU:HD21	2.06	0.55
3:A:44:ARG:HE	3:A:56:GLY:HA2	1.71	0.55
3:A:218:ARG:HG2	3:A:219:LYS:N	2.21	0.55
6:D:38:GLU:HG2	6:D:57:LEU:HD11	1.88	0.55
14:L:43:ILE:HG23	14:L:49:GLN:O	2.06	0.55
21:S:100:THR:CG2	21:S:138:VAL:HG11	2.36	0.55
1:X:794:A:H5'	3:A:219:LYS:NZ	2.22	0.55
1:X:822:G:O2'	1:X:823:U:H5'	2.07	0.55
1:X:1974:U:H2'	1:X:1975:G:H5'	1.87	0.55
2:Y:50:U:H2'	2:Y:51:G:C8	2.41	0.55
13:K:79:VAL:HG13	13:K:80:MET:N	2.21	0.55
13:K:84:ALA:HB3	13:K:85:PRO:CD	2.32	0.55
20:R:48:VAL:HG12	20:R:50:GLY:H	1.72	0.55
21:S:95:SER:HB3	21:S:119:ASN:HD21	1.72	0.55
21:S:120:LEU:HD23	21:S:120:LEU:C	2.27	0.55
29:3:8:LYS:HG3	29:3:12:ARG:HH12	1.71	0.55
1:X:218:A:C8	1:X:220:U:O2	2.60	0.55
1:X:1031:C:H1'	1:X:1032:A:OP2	2.06	0.55
1:X:1655:C:H4'	1:X:2689:C:O2	2.06	0.55
1:X:1699:A:H2'	1:X:1700:C:C6	2.41	0.55
1:X:2728:A:C2	1:X:2737:A:C6	2.95	0.55
11:I:31:GLY:HA3	11:I:34:HIS:ND1	2.22	0.55
28:2:34:ARG:NH1	28:2:42:LEU:HG	2.21	0.55
1:X:115:G:C6	1:X:117:A:N6	2.75	0.55
1:X:174:A:H2	1:X:2413:A:N6	2.05	0.55
1:X:839:U:OP1	1:X:2408:G:OP1	2.24	0.55
1:X:1673:C:H42	1:X:1987:G:H1	1.54	0.55
1:X:1744:G:H2'	1:X:1746:A:OP2	2.07	0.55
1:X:2013:A:H4'	1:X:2014:A:C8	2.41	0.55
1:X:2013:A:H4'	1:X:2014:A:H8	1.71	0.55
1:X:2453:C:H5'	1:X:2454:C:OP2	2.07	0.55
1:X:2705:A:C8	1:X:2707:G:C5	2.95	0.55
3:A:252:GLY:HA3	3:A:256:LYS:NZ	2.21	0.55
9:G:103:TYR:CE1	9:G:111:LYS:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:29:ILE:HG12	10:H:30:GLY:N	2.19	0.55
15:M:66:PHE:CD2	15:M:83:PHE:CE1	2.94	0.55
22:T:65:GLY:HA3	22:T:81:ILE:HG22	1.88	0.55
1:X:807:A:H2'	1:X:808:C:C6	2.42	0.55
1:X:1141:U:H3	1:X:2008:C:H5"	1.72	0.55
1:X:1507:A:O4'	3:A:100:ASP:HB3	2.06	0.55
1:X:2375:G:H2'	1:X:2376:G:H8	1.72	0.55
1:X:2404:A:C4'	1:X:2405:A:OP2	2.55	0.55
1:X:2821:G:C6	1:X:2846:G:N2	2.75	0.55
2:Y:8:C:H1'	14:L:39:TYR:OH	2.07	0.55
14:L:42:ILE:HD13	14:L:43:ILE:N	2.22	0.55
20:R:15:HIS:CE1	20:R:16:PHE:CD2	2.94	0.55
1:X:2235:G:N2	1:X:2254:C:N4	2.55	0.55
17:O:6:GLN:O	17:O:7:THR:OG1	2.19	0.55
1:X:958:G:H2'	1:X:959:C:C6	2.42	0.54
1:X:1182:U:O2'	1:X:1183:C:H5"	2.07	0.54
1:X:1272:G:H2'	1:X:1273:G:C8	2.42	0.54
1:X:1447:U:H1'	1:X:1577:G:N2	2.22	0.54
1:X:1769:U:H5	1:X:1775:A:C2	2.25	0.54
1:X:2477:C:OP2	1:X:2478:C:OP2	2.26	0.54
1:X:2557:G:N7	4:B:140:SER:HB3	2.22	0.54
1:X:2751:C:H2'	1:X:2752:C:C6	2.42	0.54
3:A:26:THR:HG22	3:A:27:LYS:N	2.21	0.54
4:B:93:VAL:C	4:B:95:ILE:H	2.10	0.54
10:H:127:VAL:HG13	10:H:133:VAL:HG21	1.88	0.54
1:X:1062:G:H4'	1:X:2732:C:O2'	2.07	0.54
1:X:2031:A:C2	1:X:2600:A:C2	2.94	0.54
1:X:2355:A:H2'	1:X:2356:A:O4'	2.07	0.54
9:G:94:LYS:HG2	9:G:117:GLU:HB2	1.89	0.54
9:G:103:TYR:CZ	9:G:111:LYS:HB2	2.42	0.54
12:J:16:GLY:O	12:J:17:ARG:HB3	2.06	0.54
19:Q:29:VAL:HG11	19:Q:38:ILE:HD11	1.89	0.54
19:Q:62:ARG:O	19:Q:70:GLY:HA3	2.07	0.54
23:U:32:ARG:H	23:U:32:ARG:NE	2.05	0.54
1:X:883:A:H5'	12:J:10:PHE:O	2.06	0.54
1:X:962:C:H42	1:X:977:G:H1	1.56	0.54
1:X:1813:A:H2'	1:X:1814:G:C8	2.43	0.54
1:X:1922:U:O2	1:X:1922:U:O4'	2.25	0.54
1:X:1981:A:O3'	1:X:2704:U:H4'	2.07	0.54
1:X:2542:U:H2'	1:X:2544:A:OP2	2.07	0.54
1:X:2660:C:C2	1:X:2704:U:O4	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2674:C:H2'	1:X:2675:U:H6	1.73	0.54
10:H:16:ALA:CB	10:H:98:ILE:HD11	2.36	0.54
25:W:13:PRO:O	25:W:17:VAL:HG23	2.07	0.54
1:X:1974:U:H2'	1:X:1975:G:C5'	2.38	0.54
1:X:1978:U:H2'	1:X:1979:C:C5	2.42	0.54
1:X:2201:G:H2'	1:X:2202:G:H8	1.72	0.54
1:X:2570:C:H2'	1:X:2571:G:C8	2.43	0.54
1:X:2791:C:O2'	1:X:2792:C:H5'	2.07	0.54
3:A:245:ARG:HA	3:A:253:LYS:HZ1	1.71	0.54
14:L:51:LEU:HD12	14:L:51:LEU:N	2.23	0.54
17:O:10:LYS:HD2	17:O:37:ALA:HB3	1.90	0.54
18:P:57:LEU:HD13	18:P:69:ALA:HA	1.89	0.54
19:Q:48:VAL:CG2	19:Q:82:LEU:HD22	2.38	0.54
20:R:106:VAL:O	20:R:107:ALA:HB2	2.06	0.54
1:X:494:A:N7	20:R:56:LYS:NZ	2.50	0.54
1:X:536:A:N6	1:X:2605:C:H4'	2.22	0.54
1:X:742:G:C4	1:X:1766:U:O2	2.61	0.54
1:X:1478:U:H2'	1:X:1479:G:C8	2.43	0.54
1:X:2044:G:N7	1:X:2482:A:O4'	2.40	0.54
1:X:2836:U:C2	1:X:2837:G:C8	2.95	0.54
2:Y:56:G:H2'	2:Y:57:U:O4'	2.08	0.54
4:B:9:ILE:HG22	15:M:13:LEU:HD11	1.90	0.54
6:D:112:ARG:H	6:D:112:ARG:HD2	1.73	0.54
16:N:17:VAL:HG21	16:N:32:TYR:CE1	2.40	0.54
18:P:37:LYS:HE2	18:P:64:ALA:CB	2.36	0.54
27:1:51:ARG:HD2	27:1:51:ARG:C	2.28	0.54
1:X:225:G:N7	1:X:227:G:N3	2.55	0.54
1:X:1076:U:OP1	8:F:86:LYS:HD3	2.07	0.54
1:X:1212:U:H2'	1:X:1213:U:C6	2.43	0.54
1:X:1356:G:N2	1:X:1418:C:C2	2.76	0.54
1:X:1607:A:H1'	1:X:1608:U:O5'	2.08	0.54
1:X:2074:U:H3'	1:X:2075:U:C5'	2.37	0.54
9:G:117:GLU:C	9:G:119:LEU:H	2.11	0.54
10:H:46:HIS:HB2	10:H:49:ASP:OD2	2.08	0.54
14:L:43:ILE:N	14:L:43:ILE:HD12	2.21	0.54
21:S:100:THR:HG23	21:S:138:VAL:CG1	2.38	0.54
1:X:456:C:OP2	16:N:2:PRO:HD3	2.08	0.54
1:X:1283:C:H5"	1:X:1284:G:O5'	2.08	0.54
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.41	0.54
1:X:1644:G:H2'	1:X:1645:U:C6	2.43	0.54
1:X:2262:C:H5'	27:1:7:ARG:NH2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2292:C:H5'	6:D:37:ASN:ND2	2.23	0.54
1:X:2616:U:H5'	4:B:44:TYR:CE1	2.43	0.54
9:G:61:ARG:HA	9:G:65:LYS:HB2	1.88	0.54
9:G:137:LYS:HG2	9:G:137:LYS:O	2.07	0.54
11:I:57:ILE:O	11:I:58:ALA:O	2.25	0.54
13:K:103:ARG:CG	13:K:104:ARG:N	2.70	0.54
14:L:33:ARG:HE	14:L:38:ILE:CB	2.21	0.54
20:R:17:LYS:O	20:R:36:VAL:HG11	2.07	0.54
23:U:17:SER:OG	23:U:45:ASN:N	2.40	0.54
27:1:9:ILE:HG22	27:1:28:ARG:HB2	1.89	0.54
27:1:14:SER:HB3	27:1:50:PHE:HZ	1.72	0.54
29:3:13:ARG:CD	29:3:25:PHE:H	2.20	0.54
1:X:623:G:N2	1:X:626:A:H2	2.05	0.54
1:X:754:G:C4	1:X:755:C:C5	2.96	0.54
1:X:999:A:OP2	25:W:8:SER:HB3	2.08	0.54
1:X:1074:G:H1	1:X:1086:C:N4	2.05	0.54
1:X:1179:A:C2	1:X:1196:G:C2	2.95	0.54
1:X:1336:G:O6	1:X:1337:G:C6	2.61	0.54
1:X:2507:U:OP1	30:4:31:LYS:HE3	2.08	0.54
1:X:2696:A:H2'	1:X:2697:G:H8	1.72	0.54
10:H:17:ARG:HE	10:H:59:ALA:HB2	1.73	0.54
10:H:29:ILE:HB	10:H:34:LEU:CD2	2.37	0.54
10:H:117:GLU:HA	10:H:120:ASP:OD2	2.08	0.54
14:L:89:PHE:O	14:L:91:ARG:NH2	2.41	0.54
16:N:25:TRP:CE3	16:N:26:GLY:N	2.75	0.54
1:X:537:C:H1'	1:X:538:A:C6	2.43	0.54
1:X:666:U:C2'	1:X:667:U:H5"	2.35	0.54
1:X:2043:A:N6	5:C:68:ARG:NH1	2.56	0.54
1:X:2837:G:H2'	1:X:2838:U:H6	1.72	0.54
16:N:8:ILE:O	16:N:12:ARG:HG3	2.08	0.54
27:1:41:ASP:HB3	27:1:47:HIS:H	1.72	0.54
1:X:26:G:C6	1:X:27:G:C6	2.96	0.54
1:X:471:A:C2	1:X:481:A:C4	2.96	0.54
1:X:699:G:O6	28:2:12:ARG:HA	2.08	0.54
1:X:1337:G:C4	1:X:1341:G:O6	2.61	0.54
4:B:116:VAL:HG22	4:B:136:ARG:CG	2.38	0.54
9:G:41:TRP:CZ3	9:G:79:PHE:CG	2.96	0.54
10:H:24:VAL:HG12	10:H:42:LYS:HG2	1.88	0.54
11:I:62:LYS:HD2	29:3:25:PHE:CE1	2.43	0.54
20:R:15:HIS:CE1	20:R:16:PHE:HD2	2.26	0.54
1:X:623:G:H3'	1:X:624:A:H5"	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:954:U:OP2	11:I:38:LYS:NZ	2.38	0.53
1:X:1607:A:C4'	1:X:1608:U:OP1	2.55	0.53
1:X:2218:G:OP1	3:A:250:PRO:HB3	2.09	0.53
3:A:44:ARG:N	3:A:44:ARG:CD	2.64	0.53
4:B:154:LYS:HG3	4:B:155:ARG:N	2.21	0.53
5:C:43:ALA:HB1	5:C:86:PRO:O	2.08	0.53
11:I:62:LYS:HD2	29:3:25:PHE:HE1	1.73	0.53
18:P:32:ARG:NH2	18:P:120:ARG:O	2.41	0.53
1:X:544:U:H2'	1:X:545:C:C6	2.43	0.53
1:X:637:G:N1	11:I:101:ARG:HD3	2.22	0.53
1:X:1265:G:H22	16:N:37:GLN:NE2	2.06	0.53
1:X:1337:G:C5	1:X:1341:G:O6	2.61	0.53
1:X:1773:C:H2'	1:X:2587:G:O2'	2.07	0.53
1:X:1810:U:C5	3:A:158:ARG:HD2	2.43	0.53
1:X:1923:U:H1'	1:X:1924:C:OP2	2.08	0.53
1:X:2045:A:O2'	1:X:2046:C:C5'	2.56	0.53
1:X:2218:G:H5'	3:A:250:PRO:CD	2.38	0.53
1:X:2554:C:O2'	4:B:140:SER:HB3	2.08	0.53
1:X:2593:A:H5'	26:Z:5:PRO:HB3	1.90	0.53
4:B:4:ILE:HG12	4:B:31:CYS:SG	2.48	0.53
7:E:107:ILE:HD11	7:E:151:VAL:HG11	1.90	0.53
12:J:15:ARG:CD	12:J:73:LYS:HG3	2.32	0.53
18:P:8:PHE:O	18:P:9:ARG:HB2	2.09	0.53
23:U:21:ARG:C	23:U:39:LYS:HD2	2.28	0.53
24:V:37:LEU:HD23	24:V:37:LEU:C	2.29	0.53
29:3:24:ALA:O	29:3:47:GLY:N	2.42	0.53
1:X:334:G:N2	5:C:162:ARG:NH2	2.55	0.53
1:X:1392:U:OP1	1:X:1392:U:C6	2.61	0.53
1:X:1420:A:H2	1:X:1612:U:O2	1.90	0.53
1:X:1944:C:H2'	1:X:1945:C:O4'	2.07	0.53
1:X:2026:C:C4	1:X:2757:G:C2	2.97	0.53
1:X:2292:C:H5'	6:D:37:ASN:HD22	1.73	0.53
1:X:2598:C:C2'	1:X:2599:U:H5'	2.37	0.53
3:A:37:ALA:HB1	3:A:63:TYR:O	2.07	0.53
1:X:38:G:N2	5:C:42:THR:HG22	2.23	0.53
1:X:652:C:N4	1:X:657:A:H61	2.06	0.53
1:X:1173:G:H4'	17:O:22:VAL:CG2	2.36	0.53
1:X:1182:U:H1'	1:X:1183:C:O5'	2.08	0.53
1:X:1407:G:H3'	1:X:1407:G:N3	2.24	0.53
1:X:1744:G:OP1	15:M:100:ARG:CD	2.57	0.53
1:X:2041:A:N1	31:X:2881:LMA:H40A	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2282:G:O2'	6:D:129:ASN:HB2	2.08	0.53
3:A:109:PRO:HB3	3:A:144:HIS:CE1	2.44	0.53
3:A:246:VAL:C	3:A:253:LYS:HD3	2.29	0.53
4:B:121:ASN:O	4:B:122:PHE:C	2.47	0.53
10:H:65:LYS:N	10:H:65:LYS:HD2	2.24	0.53
15:M:27:PHE:HB3	15:M:93:ILE:HD12	1.90	0.53
15:M:34:ARG:HE	15:M:91:VAL:HG22	1.72	0.53
18:P:106:LEU:HD23	18:P:106:LEU:O	2.08	0.53
20:R:44:GLN:O	20:R:77:HIS:HA	2.08	0.53
21:S:130:ILE:N	21:S:130:ILE:HD12	2.23	0.53
24:V:31:GLN:HA	24:V:34:ALA:HB3	1.90	0.53
1:X:99:U:H3'	1:X:100:G:H5"	1.90	0.53
1:X:224:G:C2	1:X:229:G:C6	2.96	0.53
1:X:559:C:H2'	1:X:560:G:O4'	2.08	0.53
1:X:867:G:C2	1:X:936:A:C2	2.96	0.53
1:X:1257:U:H2'	1:X:1258:G:C8	2.44	0.53
1:X:1677:C:H42	1:X:1983:G:H1	1.56	0.53
6:D:104:ILE:HD13	6:D:174:GLY:HA3	1.91	0.53
9:G:96:ASP:O	9:G:98:LYS:N	2.41	0.53
12:J:40:PRO:HB3	12:J:99:LYS:NZ	2.23	0.53
27:1:9:ILE:HG22	27:1:28:ARG:CB	2.37	0.53
27:1:11:LYS:N	27:1:11:LYS:HD2	2.24	0.53
1:X:57:G:OP1	19:Q:74:ASP:HB2	2.09	0.53
1:X:589:C:H4'	16:N:31:GLN:NE2	2.24	0.53
1:X:673:G:H2'	1:X:674:U:C6	2.43	0.53
1:X:2217:G:H2'	1:X:2217:G:N3	2.23	0.53
1:X:2366:U:H1'	22:T:41:ARG:NH1	2.24	0.53
1:X:2392:G:H2'	1:X:2393:G:H8	1.74	0.53
1:X:2664:G:C6	1:X:2705:A:N6	2.76	0.53
13:K:28:LEU:HD21	13:K:115:LEU:HD21	1.90	0.53
13:K:55:ALA:HB2	13:K:66:VAL:HG21	1.91	0.53
13:K:87:TYR:OH	13:K:115:LEU:HB3	2.08	0.53
14:L:37:HIS:O	14:L:37:HIS:CG	2.61	0.53
14:L:42:ILE:O	14:L:50:THR:HG23	2.08	0.53
1:X:668:A:H2'	1:X:669:G:O4'	2.09	0.53
1:X:999:A:H5"	25:W:8:SER:CB	2.38	0.53
1:X:1002:C:O5'	1:X:1002:C:H6	1.92	0.53
1:X:1544:A:C2	1:X:1560:A:C2	2.96	0.53
1:X:1810:U:C6	3:A:158:ARG:HD2	2.44	0.53
10:H:19:ILE:O	10:H:19:ILE:HG13	2.08	0.53
17:O:68:LYS:HD2	17:O:69:ILE:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:70:TYR:CD2	17:O:83:ARG:NH1	2.73	0.53
28:2:42:LEU:CD1	28:2:42:LEU:H	2.22	0.53
29:3:41:ILE:HG22	29:3:42:ARG:HD3	1.91	0.53
1:X:1357:U:C2'	1:X:1358:C:OP1	2.56	0.53
1:X:2039:G:C8	1:X:2556:A:C6	2.97	0.53
1:X:2598:C:H4'	4:B:150:VAL:HG22	1.91	0.53
4:B:31:CYS:HB3	4:B:49:ILE:CG1	2.39	0.53
11:I:49:PHE:CD1	11:I:50:GLU:N	2.76	0.53
12:J:99:LYS:CE	12:J:100:PRO:HD2	2.38	0.53
1:X:304:A:C6	1:X:359:G:N2	2.77	0.53
1:X:500:G:H2'	1:X:501:G:O4'	2.09	0.53
1:X:591:G:H1	1:X:1271:C:H42	1.57	0.53
1:X:746:G:O6	1:X:774:A:C8	2.62	0.53
1:X:760:U:O2'	1:X:761:G:P	2.66	0.53
1:X:1433:A:H62	1:X:1435:G:C1'	2.22	0.53
1:X:1888:C:H2'	1:X:1913:G:N7	2.23	0.53
1:X:1938:U:H4'	1:X:1939:U:OP2	2.08	0.53
1:X:1949:A:H61	1:X:2581:A:H62	1.56	0.53
1:X:2486:C:C2	1:X:2562:G:C2	2.96	0.53
4:B:134:TRP:CD1	4:B:134:TRP:N	2.74	0.53
7:E:137:ASP:HB3	7:E:140:LEU:HD12	1.91	0.53
10:H:51:ILE:HD12	10:H:52:VAL:O	2.08	0.53
21:S:149:ALA:O	21:S:160:LEU:HD11	2.08	0.53
1:X:455:A:H1'	1:X:1215:A:O4'	2.09	0.53
1:X:474:G:N2	1:X:477:A:OP2	2.38	0.53
1:X:518:A:N6	18:P:30:TYR:CD1	2.77	0.53
1:X:746:G:C5	1:X:774:A:C5	2.97	0.53
1:X:1257:U:H2'	1:X:1258:G:H8	1.73	0.53
1:X:1370:U:H2'	1:X:1371:G:O4'	2.08	0.53
1:X:1399:C:O2'	1:X:1400:A:H5'	2.09	0.53
1:X:1688:U:O2'	1:X:1690:U:H5	1.90	0.53
1:X:2311:U:C4'	1:X:2315:A:N6	2.71	0.53
3:A:66:ILE:HD11	3:A:107:LEU:HD12	1.89	0.53
3:A:73:LYS:HE2	3:A:98:TYR:CD2	2.44	0.53
5:C:74:VAL:HG23	5:C:76:THR:H	1.74	0.53
9:G:100:TYR:CB	9:G:116:ARG:HH11	2.08	0.53
13:K:103:ARG:CG	13:K:104:ARG:H	2.22	0.53
18:P:25:PHE:CD1	18:P:127:ILE:HD11	2.40	0.53
1:X:1174:G:C2	1:X:1175:A:C5	2.96	0.52
13:K:90:ARG:HD2	13:K:94:TYR:HB2	1.92	0.52
1:X:75:C:N3	1:X:109:A:C2	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1053:G:H1'	1:X:1054:C:O5'	2.08	0.52
1:X:1145:C:C6	1:X:1147:G:OP2	2.62	0.52
1:X:1218:C:H4'	11:I:13:ARG:NH1	2.23	0.52
1:X:2528:G:C2	1:X:2529:G:N7	2.77	0.52
3:A:28:LYS:NZ	3:A:30:PRO:HG3	2.23	0.52
4:B:116:VAL:H	4:B:136:ARG:CD	2.22	0.52
10:H:2:ILE:CB	10:H:45:ALA:HB3	2.37	0.52
12:J:43:ILE:HG13	12:J:98:VAL:HG21	1.91	0.52
24:V:17:GLU:HB3	24:V:21:ARG:NH1	2.24	0.52
1:X:463:C:C2	1:X:465:C:C5	2.97	0.52
1:X:762:A:H2	1:X:766:A:O2'	1.91	0.52
1:X:810:U:H2'	1:X:811:G:O4'	2.09	0.52
1:X:1429:A:H1'	1:X:1603:A:C6	2.43	0.52
2:Y:9:G:H5"	14:L:32:TYR:CE1	2.44	0.52
9:G:61:ARG:NE	9:G:65:LYS:HD2	2.24	0.52
10:H:26:ASN:HB3	10:H:38:GLY:H	1.73	0.52
11:I:43:ALA:O	11:I:45:LYS:CB	2.57	0.52
28:2:25:LYS:NZ	28:2:28:ARG:HG3	2.24	0.52
30:4:15:LYS:HB2	30:4:26:ILE:HG13	1.90	0.52
1:X:758:G:C2'	1:X:759:C:OP1	2.57	0.52
1:X:1010:U:O2'	1:X:1011:A:H5'	2.09	0.52
1:X:1746:A:C2	1:X:2696:A:H1'	2.44	0.52
1:X:1811:A:H2'	3:A:179:PRO:HG2	1.91	0.52
1:X:2468:G:O2'	1:X:2469:G:H5'	2.09	0.52
1:X:2664:G:N2	1:X:2665:G:H1'	2.23	0.52
3:A:38:LEU:HB3	3:A:39:PRO:HD2	1.92	0.52
3:A:247:PRO:C	3:A:249:THR:H	2.12	0.52
12:J:64:LYS:HD3	12:J:108:ALA:O	2.09	0.52
12:J:69:ILE:HD13	12:J:104:MET:HB3	1.90	0.52
18:P:80:LEU:HD11	18:P:87:GLU:HB3	1.91	0.52
1:X:513:A:C6	1:X:516:G:C6	2.97	0.52
1:X:1433:A:C4	1:X:1595:A:C2	2.98	0.52
1:X:1976:U:C5	1:X:1977:C:C5	2.97	0.52
1:X:2340:C:OP1	29:3:27:SER:N	2.36	0.52
1:X:2815:C:H42	1:X:2852:G:H1	1.57	0.52
6:D:40:LEU:HD11	6:D:50:ILE:HA	1.91	0.52
16:N:24:PHE:CB	16:N:29:SER:HB3	2.40	0.52
17:O:13:ARG:HD3	17:O:16:GLU:HB2	1.90	0.52
18:P:110:ALA:O	18:P:111:ARG:HB2	2.08	0.52
21:S:47:SER:OG	21:S:48:THR:N	2.42	0.52
1:X:538:A:H3'	9:G:142:ARG:HH22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:793:G:H21	1:X:796:A:H62	1.57	0.52
1:X:795:A:H5'	1:X:796:A:C2	2.44	0.52
1:X:968:C:N4	1:X:970:A:C5	2.78	0.52
1:X:2289:A:C2	6:D:79:LEU:HD11	2.34	0.52
3:A:78:ALA:HB2	3:A:98:TYR:CD1	2.43	0.52
10:H:9:ASP:HB2	10:H:95:ALA:HB2	1.90	0.52
16:N:16:LYS:O	16:N:19:LYS:HG2	2.09	0.52
28:2:19:ARG:NH1	28:2:19:ARG:HB2	2.24	0.52
1:X:15:G:H4'	26:Z:21:SER:HB2	1.91	0.52
1:X:659:G:H1'	29:3:46:LYS:HG3	1.92	0.52
1:X:983:G:H3'	1:X:984:A:C5'	2.39	0.52
1:X:1867:A:O2'	1:X:1868:A:C8	2.63	0.52
1:X:1976:U:C5'	4:B:128:SER:HB3	2.39	0.52
9:G:162:LYS:N	9:G:163:PRO:CD	2.72	0.52
13:K:85:PRO:O	13:K:88:ALA:HB2	2.10	0.52
16:N:7:GLY:O	16:N:9:VAL:HG23	2.10	0.52
16:N:11:ARG:HB3	16:N:15:LYS:HZ1	1.75	0.52
1:X:399:G:H4'	23:U:21:ARG:HH12	1.75	0.52
1:X:1355:A:HO2'	1:X:1357:U:P	2.32	0.52
1:X:1920:A:H5"	1:X:1921:A:OP2	2.09	0.52
1:X:1963:G:O2'	1:X:1965:U:OP2	2.28	0.52
1:X:2234:G:H2'	1:X:2235:G:O4'	2.09	0.52
1:X:2422:C:O2'	1:X:2423:G:H5'	2.10	0.52
1:X:2736:U:H3	1:X:2738:A:N6	1.89	0.52
3:A:148:LEU:CD2	3:A:156:LEU:HD11	2.40	0.52
4:B:115:GLY:HA3	4:B:136:ARG:HD2	1.92	0.52
19:Q:29:VAL:HG11	19:Q:38:ILE:CD1	2.40	0.52
22:T:45:PHE:HA	22:T:77:ARG:HB2	1.92	0.52
1:X:13:A:N3	1:X:15:G:O6	2.43	0.52
1:X:57:G:N3	1:X:69:G:N2	2.58	0.52
1:X:203:G:H1'	1:X:205:A:H61	1.75	0.52
1:X:215:G:H21	1:X:632:A:H8	1.57	0.52
1:X:537:C:O2'	1:X:538:A:C4	2.61	0.52
1:X:689:A:H1'	1:X:2422:C:O4'	2.10	0.52
1:X:941:U:H2'	1:X:942:U:O4'	2.09	0.52
1:X:1224:A:H4'	1:X:1225:G:OP2	2.10	0.52
1:X:2264:C:OP2	27:1:28:ARG:HD3	2.10	0.52
1:X:2706:U:OP1	1:X:2706:U:C6	2.63	0.52
1:X:2722:C:OP1	30:4:35:ARG:HD2	2.10	0.52
1:X:2736:U:C5'	30:4:19:ARG:HG2	2.40	0.52
4:B:131:SER:HB2	4:B:134:TRP:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:45:ILE:O	18:P:48:LYS:HG2	2.10	0.52
21:S:128:ARG:HG3	21:S:129:ARG:HG3	1.91	0.52
1:X:603:C:H5"	29:3:62:LEU:HD13	1.92	0.52
1:X:659:G:O2'	1:X:660:G:H5'	2.09	0.52
1:X:1255:A:H2'	1:X:1256:C:C6	2.44	0.52
1:X:1290:A:H5"	13:K:40:LYS:HZ3	1.75	0.52
1:X:1467:U:H3'	1:X:1467:U:H6	1.74	0.52
1:X:1505:U:O2	1:X:1506:C:H5	1.92	0.52
1:X:2180:U:H5	1:X:2203:G:C5	2.28	0.52
2:Y:9:G:H21	14:L:41:GLN:HE22	1.58	0.52
2:Y:44:C:H42	6:D:88:LYS:NZ	2.07	0.52
6:D:4:LEU:CG	6:D:5:LYS:H	2.23	0.52
6:D:36:VAL:HB	6:D:89:VAL:HB	1.90	0.52
21:S:134:LEU:HD21	21:S:152:ILE:HG21	1.91	0.52
27:1:51:ARG:HD2	27:1:51:ARG:O	2.10	0.52
28:2:19:ARG:HB2	28:2:19:ARG:CZ	2.40	0.52
1:X:178:C:OP2	23:U:40:ARG:CZ	2.58	0.51
1:X:787:A:H5"	3:A:49:ARG:NH2	2.26	0.51
1:X:882:C:H42	1:X:920:G:H1	1.59	0.51
1:X:1351:G:O2'	1:X:1352:G:H5'	2.10	0.51
1:X:2839:G:H2'	1:X:2840:U:C6	2.46	0.51
1:X:540:G:C6	1:X:2005:U:H5"	2.45	0.51
1:X:613:A:O4'	1:X:668:A:H2	1.92	0.51
1:X:652:C:H42	1:X:657:A:N6	2.06	0.51
1:X:2033:C:N4	1:X:2034:A:C6	2.78	0.51
1:X:2338:C:H2'	1:X:2339:A:O4'	2.09	0.51
1:X:2382:C:N4	1:X:2393:G:H1	2.08	0.51
1:X:2457:A:N7	1:X:2458:U:C5	2.78	0.51
1:X:2674:C:H2'	1:X:2675:U:C6	2.46	0.51
1:X:2782:G:C2'	1:X:2783:U:O5'	2.57	0.51
16:N:79:PHE:O	16:N:83:LEU:HD13	2.11	0.51
17:O:66:GLY:O	17:O:87:ARG:NH2	2.43	0.51
20:R:93:ARG:O	20:R:94:VAL:C	2.48	0.51
24:V:2:LYS:CG	24:V:3:PRO:HD3	2.40	0.51
27:1:11:LYS:HD2	27:1:11:LYS:H	1.75	0.51
1:X:618:A:C2	1:X:632:A:C5	2.99	0.51
1:X:753:U:H2'	1:X:754:G:H8	1.76	0.51
1:X:1644:G:H2'	1:X:1645:U:H6	1.75	0.51
1:X:1724:C:N3	1:X:1747:G:C6	2.78	0.51
1:X:2368:G:H5"	1:X:2369:U:O4'	2.10	0.51
9:G:95:LEU:HD21	9:G:117:GLU:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:32:ARG:HH22	17:O:82:ARG:HE	1.58	0.51
1:X:356:A:H2'	1:X:357:A:C8	2.46	0.51
1:X:542:A:H2'	16:N:28:ARG:HE	1.73	0.51
1:X:1923:U:OP2	1:X:2582:G:N2	2.35	0.51
1:X:2314:A:O2'	1:X:2315:A:C8	2.64	0.51
1:X:2424:G:C2'	1:X:2425:G:H5'	2.40	0.51
3:A:22:PHE:O	3:A:209:LYS:HG3	2.11	0.51
4:B:188:ILE:CG2	4:B:189:PRO:CD	2.88	0.51
20:R:16:PHE:CZ	20:R:46:VAL:HG22	2.44	0.51
24:V:6:MET:CE	24:V:56:VAL:HG21	2.41	0.51
1:X:219:G:C2'	1:X:220:U:OP2	2.59	0.51
1:X:469:G:H3'	28:2:39:ARG:O	2.10	0.51
1:X:525:A:C2'	1:X:526:C:H5'	2.40	0.51
1:X:778:G:H2'	1:X:779:U:H6	1.75	0.51
1:X:1332:G:O6	1:X:1333:G:O6	2.28	0.51
1:X:1685:A:H4'	1:X:1686:A:O5'	2.11	0.51
1:X:1941:C:C2'	1:X:1942:G:H5'	2.41	0.51
1:X:2046:C:O2	1:X:2430:A:C2	2.64	0.51
1:X:2238:G:C2	1:X:2261:G:C6	2.98	0.51
1:X:2426:G:C5	1:X:2479:U:C5	2.99	0.51
1:X:2623:A:C2'	1:X:2624:G:H5'	2.41	0.51
6:D:80:ARG:H	6:D:80:ARG:HD2	1.75	0.51
9:G:58:ILE:HG23	9:G:80:VAL:HG11	1.92	0.51
12:J:96:SER:O	12:J:98:VAL:HG23	2.11	0.51
28:2:25:LYS:HZ2	28:2:28:ARG:HG3	1.75	0.51
1:X:1781:C:C6	1:X:1781:C:H5'	2.46	0.51
1:X:2629:U:H2'	1:X:2630:C:H6	1.76	0.51
1:X:2653:A:O3'	10:H:42:LYS:HA	2.11	0.51
7:E:90:ARG:NH2	7:E:163:ARG:HH12	2.08	0.51
11:I:57:ILE:HG22	11:I:58:ALA:N	2.25	0.51
16:N:81:ASN:ND2	16:N:117:ARG:NH2	2.58	0.51
27:1:8:ILE:H	27:1:8:ILE:CD1	2.23	0.51
1:X:48:A:H8	1:X:50:G:H21	1.57	0.51
1:X:121:G:H2'	1:X:122:G:O4'	2.10	0.51
1:X:603:C:C5'	29:3:62:LEU:HD22	2.40	0.51
1:X:626:A:O2'	5:C:176:ASN:HB2	2.10	0.51
1:X:1496:G:O2'	1:X:1497:C:H5"	2.10	0.51
1:X:1787:U:H2'	1:X:1788:C:C6	2.46	0.51
1:X:2014:A:C6	1:X:2477:C:H1'	2.45	0.51
5:C:45:THR:HG21	5:C:86:PRO:HD2	1.93	0.51
11:I:85:ASP:HA	11:I:116:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:29:LEU:HD23	14:L:89:PHE:CE1	2.45	0.51
14:L:79:ALA:HB1	14:L:84:ILE:HB	1.92	0.51
24:V:49:GLU:O	24:V:53:LEU:HG	2.11	0.51
28:2:19:ARG:O	28:2:23:LYS:HG3	2.09	0.51
1:X:75:C:C2	1:X:109:A:H2	2.28	0.51
1:X:303:C:N3	1:X:360:A:H2	2.08	0.51
1:X:746:G:C8	1:X:774:A:N6	2.79	0.51
1:X:2033:C:C4	1:X:2034:A:C6	2.99	0.51
5:C:137:ALA:HB1	5:C:142:LEU:CB	2.41	0.51
10:H:14:SER:OG	10:H:98:ILE:HD12	2.11	0.51
11:I:49:PHE:CZ	29:3:59:LYS:HE3	2.46	0.51
13:K:103:ARG:HG3	13:K:104:ARG:H	1.76	0.51
18:P:126:ILE:HD12	18:P:127:ILE:N	2.25	0.51
1:X:62:U:H4'	1:X:63:A:OP1	2.10	0.51
1:X:350:U:H6	1:X:350:U:O5'	1.94	0.51
1:X:746:G:N7	1:X:774:A:N7	2.58	0.51
1:X:1607:A:H4'	1:X:1608:U:OP1	2.11	0.51
1:X:2617:G:O2'	1:X:2618:A:H8	1.93	0.51
1:X:2806:G:O4'	1:X:2858:A:C2	2.63	0.51
6:D:34:ILE:HD12	6:D:156:ILE:HG12	1.92	0.51
10:H:3:MET:O	10:H:6:SER:HB2	2.11	0.51
11:I:57:ILE:HG22	29:3:12:ARG:NH2	2.25	0.51
15:M:75:GLU:O	15:M:77:VAL:HG23	2.10	0.51
20:R:18:LYS:HD3	20:R:18:LYS:N	2.13	0.51
1:X:330:C:H2'	1:X:331:U:O4'	2.11	0.51
1:X:459:A:H1'	1:X:461:A:N6	2.26	0.51
1:X:482:A:C6	1:X:483:A:C2	2.99	0.51
1:X:2310:G:H4'	22:T:43:THR:N	2.25	0.51
1:X:2329:C:N4	1:X:2330:G:C6	2.79	0.51
1:X:2364:C:H2'	1:X:2365:U:C6	2.46	0.51
3:A:247:PRO:O	3:A:249:THR:N	2.44	0.51
4:B:84:PHE:CE2	4:B:86:PRO:CD	2.94	0.51
5:C:117:LEU:HD23	5:C:118:VAL:N	2.26	0.51
13:K:69:ASP:O	13:K:71:HIS:ND1	2.44	0.51
21:S:94:VAL:HG23	21:S:125:PRO:HG3	1.93	0.51
26:Z:3:LYS:HB3	26:Z:5:PRO:HD2	1.93	0.51
1:X:558:G:H3'	1:X:558:G:N3	2.26	0.50
1:X:751:G:O2'	1:X:752:G:O5'	2.29	0.50
1:X:838:A:H4'	1:X:2407:G:C5	2.47	0.50
1:X:1069:G:H3'	1:X:1070:G:H5"	1.92	0.50
1:X:1223:G:C5'	1:X:1224:A:H3'	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1300:A:C5'	13:K:103:ARG:HD2	2.41	0.50
1:X:1631:C:H5	1:X:1633:C:C2	2.29	0.50
1:X:1744:G:OP1	15:M:100:ARG:HD2	2.10	0.50
1:X:2238:G:N1	1:X:2261:G:C6	2.79	0.50
1:X:2475:C:OP1	12:J:83:ARG:HB3	2.11	0.50
1:X:2705:A:C4'	1:X:2706:U:OP1	2.59	0.50
4:B:78:LEU:O	4:B:79:ARG:CD	2.59	0.50
4:B:181:LEU:HD13	15:M:16:ILE:HD11	1.93	0.50
5:C:48:ARG:HB2	5:C:51:VAL:HG22	1.93	0.50
5:C:111:ARG:O	5:C:116:LYS:HB3	2.11	0.50
5:C:130:THR:O	5:C:133:PHE:HB3	2.10	0.50
17:O:80:TYR:HE2	17:O:82:ARG:CZ	2.24	0.50
1:X:538:A:C2	1:X:2025:A:C5	3.00	0.50
1:X:877:G:C6	1:X:878:C:N4	2.79	0.50
1:X:1404:C:H41	1:X:1407:G:P	2.34	0.50
1:X:2016:A:C5	1:X:2019:C:N4	2.80	0.50
1:X:2210:C:OP1	23:U:45:ASN:HA	2.11	0.50
1:X:2265:A:P	27:1:28:ARG:HD2	2.51	0.50
1:X:2329:C:H3'	1:X:2329:C:H6	1.76	0.50
1:X:2373:C:C5	1:X:2374:C:C5	2.99	0.50
1:X:2375:G:H4'	23:U:32:ARG:O	2.11	0.50
1:X:2634:G:H2'	1:X:2643:G:O6	2.11	0.50
3:A:71:ARG:NH2	3:A:150:PRO:HA	2.25	0.50
7:E:96:ALA:HB2	7:E:105:MET:HE1	1.92	0.50
15:M:104:LEU:C	15:M:106:TYR:H	2.13	0.50
16:N:61:TRP:CZ3	16:N:94:VAL:N	2.75	0.50
18:P:41:VAL:O	18:P:44:VAL:CG2	2.58	0.50
1:X:95:G:H4'	24:V:41:HIS:CG	2.46	0.50
1:X:789:G:C2	1:X:2220:A:OP1	2.64	0.50
1:X:1692:C:C5	1:X:1693:A:C5	2.98	0.50
1:X:2180:U:O4	1:X:2203:G:H2'	2.11	0.50
1:X:2262:C:OP1	27:1:3:LYS:HB3	2.10	0.50
1:X:2372:A:OP1	11:I:61:PRO:HB3	2.12	0.50
1:X:2379:G:N2	1:X:2380:U:O2	2.44	0.50
1:X:2659:C:C5'	4:B:189:PRO:HA	2.37	0.50
4:B:20:ALA:HB2	10:H:85:ASP:O	2.11	0.50
11:I:58:ALA:C	11:I:60:LEU:H	2.14	0.50
18:P:66:GLU:HB3	18:P:67:PRO:CD	2.32	0.50
21:S:121:GLN:O	21:S:161:ALA:HB3	2.10	0.50
1:X:573:C:H2'	1:X:574:C:H6	1.77	0.50
1:X:633:G:H2'	1:X:634:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:765:C:C5	1:X:1772:C:C2	2.99	0.50
1:X:1020:A:H4'	16:N:59:ARG:HG3	1.92	0.50
1:X:1324:G:HO2'	1:X:1325:U:H5	1.60	0.50
1:X:1787:U:H4'	3:A:255:THR:H	1.76	0.50
1:X:1945:C:O2'	1:X:1946:U:C5	2.65	0.50
1:X:2598:C:H5'	4:B:150:VAL:O	2.11	0.50
1:X:2796:A:O3'	4:B:162:MET:HE1	2.12	0.50
4:B:61:LYS:N	4:B:62:PRO:CD	2.74	0.50
11:I:61:PRO:HG3	29:3:27:SER:HA	1.93	0.50
15:M:25:PRO:O	15:M:27:PHE:CD2	2.64	0.50
16:N:25:TRP:CE3	16:N:26:GLY:HA3	2.47	0.50
1:X:465:C:O2	1:X:467:U:C6	2.65	0.50
1:X:958:G:H2'	1:X:959:C:H6	1.76	0.50
1:X:966:A:N6	1:X:967:G:C6	2.80	0.50
1:X:1050:G:H2'	1:X:1051:U:H5'	1.93	0.50
1:X:1145:C:C5	1:X:1147:G:P	3.05	0.50
1:X:1987:G:C6	1:X:1988:A:C5	3.00	0.50
1:X:2562:G:C6	1:X:2563:U:N3	2.79	0.50
31:X:2881:LMA:H35	31:X:2881:LMA:C37	2.30	0.50
3:A:95:LEU:O	3:A:95:LEU:HG	2.11	0.50
25:W:40:VAL:HA	25:W:43:MET:CG	2.41	0.50
1:X:562:G:H2'	1:X:563:U:O4'	2.11	0.50
1:X:1007:A:N6	1:X:1171:A:C6	2.79	0.50
1:X:1354:A:O3'	19:Q:54:SER:HB2	2.12	0.50
1:X:2729:A:C6	1:X:2730:A:N6	2.80	0.50
31:X:2881:LMA:O55	31:X:2881:LMA:H57	2.11	0.50
4:B:188:ILE:CG2	4:B:189:PRO:HD2	2.41	0.50
15:M:11:GLU:HG3	15:M:14:ARG:NH1	2.18	0.50
18:P:95:ALA:HB2	18:P:126:ILE:CD1	2.37	0.50
20:R:23:ILE:HD12	20:R:23:ILE:O	2.11	0.50
1:X:459:A:N6	1:X:484:G:H1'	2.27	0.50
1:X:1629:G:C6	1:X:1633:C:C5	2.99	0.50
1:X:2016:A:C6	1:X:2019:C:C4	2.99	0.50
5:C:48:ARG:O	5:C:51:VAL:HG22	2.11	0.50
6:D:134:GLU:HG2	6:D:136:LEU:H	1.76	0.50
18:P:87:GLU:HA	18:P:90:LEU:CG	2.39	0.50
21:S:88:TYR:C	21:S:127:PRO:HG2	2.31	0.50
27:1:39:LYS:HZ3	27:1:41:ASP:HB3	1.76	0.50
1:X:158:A:H2	1:X:447:U:O2'	1.95	0.50
1:X:841:G:H4'	1:X:844:G:N1	2.27	0.50
1:X:986:A:C2	1:X:1001:A:C8	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1457:A:C2	1:X:1565:G:C2	2.99	0.50
1:X:2409:A:O2'	1:X:2410:U:C5	2.65	0.50
1:X:2722:C:H2'	1:X:2723:C:H6	1.76	0.50
6:D:106:ILE:HG21	6:D:139:PRO:HB3	1.94	0.50
7:E:94:PHE:CG	7:E:107:ILE:HG22	2.46	0.50
14:L:14:ARG:O	14:L:18:ARG:HB2	2.12	0.50
23:U:66:ALA:O	23:U:70:LEU:HB2	2.12	0.50
26:Z:52:TYR:O	26:Z:53:ASP:CB	2.58	0.50
1:X:320:A:N3	1:X:340:G:O2'	2.42	0.50
1:X:588:G:N2	1:X:1275:A:C4	2.80	0.50
1:X:642:A:O2'	11:I:65:PHE:HB3	2.12	0.50
1:X:795:A:C2	3:A:227:MET:HE2	2.47	0.50
1:X:2551:A:H62	4:B:145:LYS:HD2	1.77	0.50
1:X:2571:G:C6	1:X:2572:U:N3	2.79	0.50
1:X:2757:G:OP2	1:X:2761:A:O2'	2.26	0.50
4:B:14:ILE:CA	15:M:20:HIS:HD2	2.14	0.50
12:J:35:LEU:HD12	12:J:131:LYS:O	2.11	0.50
13:K:63:ARG:HA	13:K:80:MET:HE1	1.94	0.50
1:X:79:G:H1	1:X:104:C:H42	1.58	0.49
1:X:754:G:C6	1:X:755:C:N4	2.80	0.49
1:X:1255:A:H2'	1:X:1256:C:H6	1.76	0.49
1:X:1469:U:H5"	1:X:1470:G:N7	2.27	0.49
1:X:1747:G:H5'	1:X:1748:U:OP1	2.12	0.49
1:X:1774:A:H5'	1:X:2587:G:H4'	1.93	0.49
1:X:2282:G:C2	1:X:2293:G:C2	3.00	0.49
3:A:43:GLY:H	3:A:44:ARG:NH1	2.10	0.49
7:E:103:LEU:HD21	7:E:105:MET:HE3	1.94	0.49
13:K:68:GLN:O	13:K:71:HIS:CE1	2.65	0.49
16:N:40:LEU:O	16:N:43:ALA:HB3	2.12	0.49
1:X:26:G:C5	1:X:27:G:C6	3.00	0.49
1:X:409:G:O3'	23:U:47:HIS:HE1	1.95	0.49
1:X:490:A:C4	1:X:492:G:O4'	2.65	0.49
1:X:537:C:H1'	1:X:538:A:N1	2.27	0.49
1:X:969:U:H4'	1:X:970:A:OP2	2.13	0.49
1:X:1056:U:H1'	1:X:1058:G:C2	2.47	0.49
1:X:1336:G:C2'	1:X:1337:G:H5'	2.39	0.49
1:X:1351:G:C2	1:X:1352:G:C4	3.01	0.49
1:X:1926:U:O4'	1:X:1928:G:H5'	2.13	0.49
1:X:2016:A:O4'	1:X:2016:A:OP2	2.30	0.49
1:X:2338:C:H42	1:X:2407:G:H1	1.60	0.49
4:B:147:PRO:O	4:B:149:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:99:VAL:O	9:G:99:VAL:HG12	2.11	0.49
11:I:80:LEU:HD13	11:I:120:VAL:HG22	1.94	0.49
11:I:94:GLU:HB2	11:I:97:ARG:HH11	1.76	0.49
15:M:104:LEU:O	15:M:106:TYR:N	2.44	0.49
18:P:34:SER:HA	18:P:120:ARG:HB2	1.94	0.49
23:U:49:LYS:HB3	23:U:61:TRP:CZ3	2.47	0.49
1:X:33:C:H4'	1:X:34:U:OP1	2.10	0.49
1:X:334:G:C3'	5:C:162:ARG:HD3	2.42	0.49
1:X:471:A:C2	1:X:481:A:C5	3.00	0.49
1:X:595:A:OP1	5:C:83:ALA:HB3	2.12	0.49
1:X:1145:C:C6	1:X:1147:G:P	3.06	0.49
1:X:2045:A:O2'	1:X:2046:C:O4'	2.30	0.49
1:X:2053:G:N2	1:X:2054:A:N3	2.61	0.49
1:X:2369:U:H5'	29:3:36:LYS:NZ	2.27	0.49
3:A:89:ARG:HG2	3:A:91:ALA:HB3	1.94	0.49
4:B:114:GLN:OE1	4:B:114:GLN:HA	2.11	0.49
5:C:14:THR:O	5:C:15:ILE:HB	2.11	0.49
5:C:148:VAL:HB	5:C:167:VAL:HG12	1.94	0.49
19:Q:5:ASP:O	19:Q:6:ILE:HB	2.12	0.49
1:X:20:C:O2'	1:X:21:A:H5'	2.12	0.49
1:X:105:G:C2'	1:X:106:G:H5'	2.42	0.49
1:X:116:A:OP2	1:X:117:A:H2'	2.12	0.49
1:X:124:A:OP2	28:2:44:VAL:CG1	2.60	0.49
1:X:346:C:H2'	1:X:347:C:C6	2.44	0.49
1:X:1976:U:H3'	1:X:1976:U:OP2	2.13	0.49
1:X:2490:U:O2	4:B:139:GLY:HA3	2.12	0.49
1:X:2499:C:H2'	1:X:2500:C:H5'	1.93	0.49
1:X:2569:A:H2'	1:X:2570:C:C6	2.47	0.49
1:X:2730:A:H5"	1:X:2731:G:OP1	2.12	0.49
5:C:14:THR:HG22	5:C:15:ILE:H	1.75	0.49
14:L:37:HIS:CD2	14:L:39:TYR:CZ	3.01	0.49
14:L:91:ARG:H	14:L:91:ARG:NE	2.11	0.49
16:N:61:TRP:HZ3	16:N:94:VAL:H	1.54	0.49
16:N:66:ASN:CB	16:N:76:TYR:HB2	2.36	0.49
18:P:19:LYS:O	18:P:20:LEU:HB3	2.12	0.49
20:R:98:ILE:HG22	20:R:99:VAL:HG13	1.94	0.49
24:V:52:GLN:O	24:V:56:VAL:HG23	2.12	0.49
1:X:173:A:O2'	1:X:818:G:O6	2.30	0.49
1:X:668:A:O2'	1:X:669:G:O4'	2.31	0.49
1:X:1202:U:H5'	17:O:78:VAL:HG22	1.93	0.49
1:X:2045:A:O2'	1:X:2046:C:O5'	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2262:C:P	27:1:7:ARG:HH22	2.36	0.49
1:X:2836:U:O2'	1:X:2837:G:H5'	2.12	0.49
5:C:28:HIS:ND1	11:I:17:LYS:HA	2.27	0.49
9:G:38:GLU:HG3	9:G:68:PRO:HB3	1.94	0.49
11:I:56:LEU:HD22	29:3:52:LYS:NZ	2.26	0.49
18:P:64:ALA:O	18:P:67:PRO:HD2	2.12	0.49
21:S:13:LYS:HG3	21:S:18:MET:HB2	1.94	0.49
29:3:14:ILE:O	29:3:14:ILE:HG12	2.13	0.49
1:X:334:G:H3'	5:C:162:ARG:HD3	1.93	0.49
1:X:525:A:C8	1:X:526:C:C6	3.01	0.49
1:X:717:G:H1'	1:X:739:G:N2	2.27	0.49
1:X:759:C:O2'	1:X:760:U:OP2	2.30	0.49
1:X:1142:G:C8	1:X:2008:C:H4'	2.48	0.49
1:X:1693:A:C2	1:X:1976:U:H5'	2.47	0.49
1:X:1997:A:H5'	18:P:115:ASN:ND2	2.27	0.49
1:X:2015:G:O4'	1:X:2015:G:OP1	2.30	0.49
4:B:188:ILE:HG23	4:B:189:PRO:HD2	1.94	0.49
6:D:4:LEU:HD22	6:D:101:GLU:HB2	1.94	0.49
7:E:127:GLU:CG	7:E:128:PRO:HD2	2.43	0.49
11:I:58:ALA:CA	29:3:12:ARG:HH21	2.23	0.49
12:J:95:VAL:HG12	12:J:96:SER:N	2.27	0.49
1:X:67:G:N2	1:X:73:A:C4	2.81	0.49
1:X:484:G:C2	1:X:485:G:C5	3.01	0.49
1:X:2044:G:N7	1:X:2480:C:H4'	2.27	0.49
1:X:2657:G:H2'	1:X:2658:A:O4'	2.12	0.49
1:X:2845:C:C6	1:X:2845:C:C3'	2.95	0.49
5:C:172:VAL:O	5:C:173:ALA:C	2.50	0.49
6:D:51:ASP:O	6:D:55:LYS:HG2	2.12	0.49
10:H:1:MET:HE2	10:H:1:MET:H3	1.76	0.49
13:K:28:LEU:C	13:K:28:LEU:CD2	2.77	0.49
25:W:16:GLN:O	25:W:20:VAL:HG23	2.13	0.49
29:3:30:ARG:HH21	29:3:31:HIS:HE1	1.60	0.49
1:X:502:A:H2'	1:X:503:G:O4'	2.12	0.49
1:X:693:A:C4	1:X:811:G:N2	2.81	0.49
1:X:705:C:H4'	3:A:42:GLY:O	2.13	0.49
1:X:725:C:H2'	1:X:726:G:C8	2.47	0.49
1:X:945:G:H2'	1:X:946:U:H6	1.76	0.49
1:X:2404:A:H4'	1:X:2405:A:OP2	2.11	0.49
1:X:2553:G:C2	1:X:2554:C:O2	2.66	0.49
1:X:2583:U:O2'	1:X:2584:U:H5'	2.12	0.49
1:X:2797:G:H2'	1:X:2798:A:H5"	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:73:C:H2'	2:Y:74:A:O4'	2.12	0.49
6:D:123:ASP:OD2	6:D:127:ASN:HB2	2.13	0.49
10:H:64:VAL:C	10:H:65:LYS:HD2	2.33	0.49
13:K:106:ASP:OD1	13:K:108:VAL:HG23	2.12	0.49
17:O:34:GLU:HB2	17:O:56:VAL:HG23	1.93	0.49
19:Q:35:LYS:O	19:Q:35:LYS:HG2	2.13	0.49
1:X:485:G:C6	1:X:520:C:N4	2.81	0.49
1:X:1096:A:H1'	1:X:1097:A:O5'	2.13	0.49
1:X:1770:U:C5	1:X:1775:A:N7	2.81	0.49
1:X:2291:U:P	6:D:71:LYS:HD2	2.53	0.49
1:X:2407:G:H21	11:I:59:ARG:HH22	1.61	0.49
4:B:4:ILE:HG12	4:B:5:LEU:H	1.78	0.49
17:O:67:LYS:HD2	17:O:68:LYS:N	2.27	0.49
29:3:13:ARG:CD	29:3:25:PHE:HD1	2.25	0.49
29:3:62:LEU:HB3	29:3:63:PRO:HD3	1.95	0.49
1:X:36:G:N2	1:X:457:C:C2	2.81	0.49
1:X:648:A:H4'	1:X:649:G:H5'	1.94	0.49
1:X:1398:G:OP1	1:X:1398:G:H4'	2.13	0.49
1:X:1811:A:H4'	1:X:1812:U:C5'	2.42	0.49
3:A:222:GLN:OE1	3:A:222:GLN:HA	2.13	0.49
4:B:183:LEU:HD21	15:M:16:ILE:HD13	1.95	0.49
4:B:188:ILE:HG23	4:B:189:PRO:CD	2.43	0.49
15:M:16:ILE:O	15:M:16:ILE:HG22	2.13	0.49
18:P:24:GLY:O	18:P:127:ILE:HA	2.13	0.49
1:X:346:C:C6	1:X:347:C:H5	2.30	0.48
1:X:596:C:H5'	5:C:84:PHE:HE1	1.78	0.48
1:X:1052:C:H42	1:X:1125:G:H1	1.58	0.48
1:X:1226:A:C8	1:X:1250:A:C2	3.01	0.48
1:X:1429:A:O2'	1:X:1430:G:H4'	2.13	0.48
1:X:1836:C:H42	1:X:1879:G:H1	1.61	0.48
1:X:2629:U:H2'	1:X:2630:C:C6	2.48	0.48
11:I:73:GLU:OE1	11:I:73:GLU:N	2.46	0.48
1:X:178:C:H2'	1:X:179:U:H6	1.78	0.48
1:X:224:G:H4'	1:X:399:G:C4	2.48	0.48
1:X:781:G:H2'	1:X:782:U:C6	2.48	0.48
1:X:874:A:H2'	1:X:875:G:O4'	2.13	0.48
1:X:1003:C:O3'	17:O:71:ILE:HD13	2.13	0.48
1:X:1032:A:C2	1:X:1034:U:C2	3.01	0.48
1:X:1054:C:H42	1:X:1123:G:H1	1.61	0.48
1:X:1629:G:C6	1:X:1633:C:C6	3.01	0.48
1:X:1685:A:C5	1:X:1691:G:C5	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1911:A:H2'	1:X:1912:G:O4'	2.12	0.48
1:X:2387:U:H2'	1:X:2388:G:H8	1.78	0.48
1:X:2622:G:H2'	1:X:2623:A:O4'	2.13	0.48
1:X:2654:A:H5'	10:H:41:ASN:HB2	1.95	0.48
1:X:2665:G:C5	1:X:2666:U:C4	3.01	0.48
1:X:2796:A:C2	1:X:2797:G:C4	3.01	0.48
4:B:116:VAL:H	4:B:136:ARG:NE	2.12	0.48
5:C:2:ALA:N	5:C:12:GLY:O	2.46	0.48
5:C:102:LEU:HD21	5:C:106:MET:HE3	1.95	0.48
10:H:19:ILE:HG22	10:H:55:VAL:HA	1.95	0.48
12:J:110:VAL:HB	12:J:114:GLN:HB2	1.94	0.48
19:Q:38:ILE:O	19:Q:42:ILE:HG22	2.13	0.48
19:Q:68:PHE:O	19:Q:69:ILE:C	2.51	0.48
24:V:2:LYS:HG3	24:V:3:PRO:HD3	1.94	0.48
25:W:5:LEU:HA	25:W:51:LEU:HD23	1.94	0.48
1:X:73:A:H3'	1:X:74:G:C5'	2.42	0.48
1:X:692:C:N4	1:X:811:G:H1	2.10	0.48
1:X:860:U:O2	1:X:860:U:C2'	2.61	0.48
1:X:1128:G:C2'	1:X:1129:A:H5"	2.42	0.48
1:X:1656:U:O2'	1:X:1657:A:H5"	2.12	0.48
1:X:1851:A:H2'	1:X:1852:G:O4'	2.12	0.48
1:X:1992:G:H1'	13:K:106:ASP:O	2.12	0.48
1:X:2695:C:O2'	1:X:2696:A:H5'	2.13	0.48
4:B:49:ILE:HG21	4:B:81:PHE:CE2	2.45	0.48
4:B:88:GLY:O	4:B:89:ASP:OD1	2.31	0.48
4:B:115:GLY:O	4:B:119:ARG:HB2	2.12	0.48
5:C:47:THR:HG23	5:C:85:GLY:H	1.78	0.48
16:N:20:ARG:HH12	17:O:83:ARG:NH2	2.11	0.48
20:R:11:ASN:O	20:R:11:ASN:ND2	2.36	0.48
27:1:38:LYS:HD3	27:1:40:TYR:HE1	1.78	0.48
1:X:465:C:O2	1:X:467:U:H6	1.96	0.48
1:X:795:A:C2	3:A:227:MET:HG2	2.49	0.48
1:X:1008:G:C2	1:X:1170:U:O2	2.66	0.48
1:X:1118:G:C2'	1:X:1119:U:H5'	2.44	0.48
1:X:1631:C:H5	1:X:1633:C:C6	2.31	0.48
1:X:1796:A:H1'	3:A:51:THR:HG23	1.94	0.48
1:X:2237:C:C4	1:X:2405:A:H5'	2.48	0.48
1:X:2299:A:H4'	1:X:2300:G:C2	2.48	0.48
10:H:113:PRO:HD3	15:M:73:PHE:HB2	1.95	0.48
11:I:86:THR:OG1	11:I:118:VAL:HG12	2.12	0.48
14:L:31:VAL:CG2	14:L:33:ARG:HG3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:25:PHE:C	18:P:25:PHE:CD2	2.87	0.48
18:P:91:PHE:CD1	18:P:129:ALA:O	2.66	0.48
19:Q:62:ARG:O	19:Q:70:GLY:CA	2.61	0.48
1:X:76:C:O4'	24:V:55:THR:HG21	2.13	0.48
1:X:573:C:H2'	1:X:574:C:C6	2.49	0.48
1:X:746:G:H3'	1:X:774:A:H61	1.78	0.48
1:X:819:C:H2'	1:X:820:U:H6	1.77	0.48
1:X:1968:G:H2'	1:X:1969:G:C8	2.45	0.48
1:X:1980:A:C2	1:X:1981:A:C5	3.01	0.48
1:X:2064:U:H5'	23:U:41:VAL:HG21	1.96	0.48
1:X:2527:G:C6	1:X:2540:A:N1	2.82	0.48
1:X:2757:G:H5"	1:X:2758:A:C5'	2.33	0.48
1:X:2762:G:N2	1:X:2763:U:C2	2.82	0.48
1:X:2800:C:C5	1:X:2801:A:C8	3.01	0.48
31:X:2881:LMA:C54	31:X:2881:LMA:C34	2.91	0.48
3:A:109:PRO:HB3	3:A:144:HIS:HE1	1.78	0.48
3:A:244:GLY:C	3:A:245:ARG:NE	2.67	0.48
4:B:44:TYR:HB2	4:B:82:ARG:HH12	1.79	0.48
4:B:116:VAL:N	4:B:136:ARG:HE	2.11	0.48
19:Q:63:LYS:HD3	19:Q:69:ILE:CA	2.43	0.48
1:X:75:C:H2'	1:X:76:C:H5'	1.94	0.48
1:X:304:A:H62	1:X:356:A:N6	2.11	0.48
1:X:334:G:H2'	5:C:162:ARG:CD	2.44	0.48
1:X:538:A:N6	1:X:2025:A:H2'	2.28	0.48
1:X:778:G:H2'	1:X:779:U:C6	2.48	0.48
1:X:1033:G:C6	1:X:1151:U:C5	3.01	0.48
1:X:1357:U:H4'	1:X:1397:A:N6	2.27	0.48
1:X:1674:C:H2'	1:X:1674:C:O2	2.14	0.48
3:A:201:GLU:HG3	3:A:203:LYS:H	1.78	0.48
4:B:105:THR:CG2	4:B:197:VAL:HB	2.44	0.48
11:I:31:GLY:C	11:I:32:ARG:HG3	2.33	0.48
23:U:32:ARG:H	23:U:32:ARG:CZ	2.27	0.48
26:Z:58:LEU:H	26:Z:58:LEU:CD1	2.24	0.48
1:X:476:G:H4'	28:2:16:HIS:CG	2.48	0.48
1:X:1560:A:C2'	1:X:1561:A:H5'	2.44	0.48
1:X:1762:C:C2	1:X:1763:G:C8	3.00	0.48
1:X:1782:A:O3'	3:A:206:VAL:O	2.31	0.48
1:X:1813:A:OP1	3:A:160:ALA:HB3	2.14	0.48
1:X:1871:G:H3'	1:X:1871:G:N3	2.28	0.48
1:X:2426:G:C8	1:X:2479:U:C6	3.02	0.48
1:X:2796:A:H5"	4:B:162:MET:HE1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2812:A:H2'	1:X:2813:G:C8	2.49	0.48
2:Y:65:A:H2'	2:Y:66:G:C8	2.48	0.48
9:G:49:VAL:HG21	9:G:170:PRO:HG2	1.95	0.48
12:J:39:GLU:HB3	12:J:128:ILE:CG2	2.43	0.48
27:1:9:ILE:HD12	27:1:26:LYS:HD2	1.94	0.48
27:1:34:LYS:HE3	27:1:34:LYS:CA	2.37	0.48
27:1:39:LYS:C	27:1:39:LYS:HD3	2.33	0.48
1:X:321:A:O2'	1:X:322:A:H2'	2.14	0.48
1:X:1283:C:H5"	1:X:1284:G:C5'	2.44	0.48
1:X:1469:U:H5	13:K:64:ARG:NH2	2.10	0.48
1:X:1774:A:N1	1:X:2566:A:H2'	2.29	0.48
1:X:1836:C:C2	1:X:1880:G:N2	2.82	0.48
6:D:79:LEU:HD12	6:D:79:LEU:N	2.29	0.48
6:D:103:LEU:HD12	6:D:107:GLY:HA3	1.95	0.48
7:E:117:PRO:HD3	7:E:123:PHE:CE1	2.49	0.48
17:O:36:LYS:HZ1	17:O:54:TYR:HB3	1.78	0.48
19:Q:19:ALA:O	19:Q:24:VAL:HB	2.13	0.48
28:2:40:HIS:O	28:2:41:GLN:CD	2.52	0.48
1:X:412:U:H2'	1:X:413:G:O4'	2.13	0.48
1:X:477:A:H4'	28:2:30:ILE:HD13	1.95	0.48
1:X:596:C:H5'	5:C:84:PHE:CE1	2.49	0.48
1:X:1482:U:H2'	1:X:1483:G:H8	1.78	0.48
1:X:2329:C:H2'	1:X:2330:G:O4'	2.14	0.48
1:X:2690:A:OP1	1:X:2692:A:OP2	2.31	0.48
1:X:2795:A:H1'	13:K:5:LYS:NZ	2.29	0.48
4:B:60:ASN:O	4:B:64:GLN:HG3	2.13	0.48
9:G:56:THR:N	9:G:134:MET:HE1	2.28	0.48
13:K:84:ALA:N	13:K:85:PRO:HD2	2.29	0.48
15:M:60:SER:HA	15:M:64:LYS:HB2	1.95	0.48
18:P:60:ILE:HA	18:P:61:PRO:HD3	1.63	0.48
20:R:22:VAL:HG12	20:R:23:ILE:N	2.28	0.48
20:R:23:ILE:HD12	20:R:23:ILE:C	2.34	0.48
28:2:40:HIS:O	28:2:41:GLN:OE1	2.31	0.48
1:X:34:U:H1'	20:R:4:PRO:HA	1.96	0.48
1:X:814:G:OP1	5:C:50:GLN:OE1	2.32	0.48
1:X:1175:A:C2	1:X:1176:U:C2	3.02	0.48
1:X:1229:C:H2'	1:X:1230:C:H6	1.79	0.48
1:X:1779:C:H2'	1:X:1780:A:H8	1.79	0.48
1:X:2192:U:C4	1:X:2193:C:C4	3.02	0.48
1:X:2265:A:H61	27:1:25:THR:HG21	1.79	0.48
1:X:2552:C:H5"	1:X:2553:G:H5"	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:50:U:H2'	2:Y:51:G:H8	1.78	0.48
7:E:107:ILE:HD11	7:E:151:VAL:CG1	2.44	0.48
14:L:33:ARG:HH21	14:L:38:ILE:HG21	1.78	0.48
15:M:103:LYS:HG3	15:M:105:TYR:CZ	2.48	0.48
21:S:104:SER:HA	21:S:139:THR:HA	1.95	0.48
23:U:23:LYS:HA	23:U:36:GLY:O	2.14	0.48
27:1:41:ASP:HB2	27:1:46:LYS:HA	1.96	0.48
1:X:224:G:H4'	1:X:399:G:C5	2.49	0.47
1:X:538:A:H5"	9:G:142:ARG:NH1	2.29	0.47
1:X:815:A:C6	1:X:816:U:C4	3.01	0.47
1:X:1223:G:C6	1:X:1250:A:N7	2.82	0.47
1:X:1441:A:H1'	1:X:1442:C:OP2	2.14	0.47
1:X:1810:U:O4	3:A:155:GLN:HG2	2.14	0.47
1:X:2273:C:H2'	1:X:2274:C:C6	2.49	0.47
1:X:2821:G:H2'	1:X:2822:U:C6	2.48	0.47
3:A:44:ARG:HH21	3:A:56:GLY:HA2	1.79	0.47
4:B:136:ARG:CG	4:B:137:ARG:N	2.75	0.47
5:C:107:ALA:HB1	5:C:180:ILE:HD13	1.96	0.47
5:C:158:ARG:O	5:C:160:ALA:N	2.47	0.47
7:E:139:GLN:O	7:E:143:GLN:HG3	2.14	0.47
11:I:32:ARG:HD2	11:I:32:ARG:O	2.14	0.47
15:M:19:ASP:C	15:M:20:HIS:ND1	2.68	0.47
16:N:7:GLY:O	16:N:8:ILE:HG12	2.14	0.47
16:N:88:ILE:HA	17:O:49:GLU:HG3	1.96	0.47
27:1:40:TYR:H	27:1:50:PHE:HB3	1.79	0.47
27:1:45:LYS:O	27:1:46:LYS:HB2	2.13	0.47
1:X:161:U:H4'	1:X:194:G:N2	2.26	0.47
1:X:308:C:H4'	20:R:95:ARG:CZ	2.44	0.47
1:X:640:C:H4'	1:X:660:G:N3	2.29	0.47
1:X:1142:G:C2	9:G:103:TYR:HD2	2.31	0.47
1:X:2285:U:C2	6:D:150:ARG:NH2	2.82	0.47
1:X:2401:A:N3	1:X:2403:C:C4	2.82	0.47
1:X:2639:A:H2'	1:X:2640:G:O4'	2.13	0.47
1:X:2860:C:H2'	1:X:2861:A:O4'	2.14	0.47
2:Y:16:U:H4'	2:Y:72:C:O2	2.14	0.47
22:T:65:GLY:HA3	22:T:81:ILE:CG2	2.44	0.47
1:X:983:G:O2'	1:X:984:A:OP1	2.32	0.47
1:X:1025:A:H2	1:X:1160:C:C2	2.32	0.47
1:X:1326:U:H4'	1:X:1345:G:H4'	1.97	0.47
1:X:1781:C:H1'	3:A:210:ALA:HB2	1.95	0.47
1:X:1979:C:O2	1:X:1980:A:H1'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2324:G:C2	1:X:2360:C:H2'	2.48	0.47
5:C:102:LEU:HD21	5:C:106:MET:HE1	1.96	0.47
7:E:137:ASP:OD2	7:E:140:LEU:HG	2.13	0.47
9:G:132:PHE:CE2	9:G:145:HIS:HB2	2.48	0.47
12:J:133:VAL:HG12	21:S:76:ARG:HE	1.80	0.47
17:O:30:GLY:O	17:O:32:LYS:HG2	2.15	0.47
20:R:106:VAL:HG23	20:R:113:THR:HG21	1.96	0.47
22:T:43:THR:HG22	22:T:46:LYS:HE2	1.96	0.47
1:X:521:U:C5	1:X:522:G:C2	3.03	0.47
1:X:1074:G:H4'	8:F:134:MET:HG3	1.97	0.47
1:X:1755:G:C6	1:X:1972:G:C2	3.01	0.47
1:X:2053:G:C2	1:X:2054:A:C4	3.01	0.47
1:X:2237:C:O2'	1:X:2406:C:OP2	2.18	0.47
1:X:2825:A:N7	1:X:2843:A:O2'	2.32	0.47
10:H:62:GLY:O	10:H:65:LYS:NZ	2.43	0.47
10:H:115:ALA:HB3	10:H:118:LEU:HD13	1.96	0.47
15:M:34:ARG:HH11	15:M:88:VAL:HG21	1.77	0.47
18:P:107:ILE:HG21	18:P:117:ILE:HG12	1.96	0.47
1:X:467:U:HO2'	1:X:468:A:P	2.37	0.47
1:X:888:G:N2	1:X:915:C:C2	2.82	0.47
1:X:977:G:O4'	1:X:2246:A:N6	2.48	0.47
1:X:1482:U:H2'	1:X:1483:G:C8	2.49	0.47
10:H:41:ASN:HB2	10:H:42:LYS:H	1.53	0.47
23:U:22:GLY:HA3	23:U:39:LYS:CG	2.44	0.47
1:X:55:A:C2	1:X:113:C:O2	2.67	0.47
1:X:193:A:C4	1:X:445:A:C2	3.03	0.47
1:X:525:A:H2'	1:X:526:C:H5'	1.96	0.47
1:X:694:G:H2'	1:X:695:G:O4'	2.15	0.47
1:X:1780:A:H5"	3:A:222:GLN:OE1	2.15	0.47
1:X:1802:A:H2'	1:X:1803:G:O4'	2.15	0.47
1:X:1813:A:H2'	1:X:1814:G:H8	1.78	0.47
1:X:1830:C:H42	1:X:1881:U:H3'	1.78	0.47
1:X:2541:U:O2'	10:H:23:ARG:NH1	2.47	0.47
1:X:2673:G:C4	1:X:2674:C:C5	3.03	0.47
3:A:45:ASN:CB	3:A:50:ILE:HA	2.39	0.47
4:B:97:ALA:HB3	4:B:100:GLU:HG3	1.96	0.47
10:H:115:ALA:HB3	10:H:118:LEU:CD1	2.45	0.47
13:K:21:ALA:HB1	13:K:47:PHE:CD2	2.50	0.47
13:K:56:LYS:O	13:K:56:LYS:HG2	2.15	0.47
17:O:10:LYS:HD2	17:O:37:ALA:CB	2.45	0.47
17:O:36:LYS:HE3	17:O:55:THR:CA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:23:ILE:HD11	20:R:81:VAL:HB	1.97	0.47
1:X:19:C:O2	1:X:532:A:C2	2.68	0.47
1:X:305:A:N1	1:X:356:A:C2	2.83	0.47
1:X:573:C:H2'	1:X:574:C:O4'	2.14	0.47
1:X:668:A:C2'	1:X:669:G:O4'	2.62	0.47
1:X:819:C:C2	1:X:820:U:C5	3.01	0.47
1:X:1087:C:OP1	8:F:90:THR:HG22	2.14	0.47
1:X:1791:C:OP1	3:A:264:ARG:HG3	2.14	0.47
1:X:1919:A:H2	1:X:1925:C:H42	1.62	0.47
1:X:1974:U:O2'	1:X:1975:G:H5"	2.14	0.47
1:X:2171:U:H4'	1:X:2171:U:OP1	2.13	0.47
1:X:2199:C:H2'	1:X:2200:G:H5'	1.96	0.47
1:X:2237:C:C3'	1:X:2238:G:H5'	2.44	0.47
1:X:2264:C:H42	1:X:2362:G:H1	1.63	0.47
1:X:2327:U:O4	1:X:2361:G:N2	2.47	0.47
1:X:2387:U:H2'	1:X:2388:G:C8	2.48	0.47
1:X:2675:U:H2'	1:X:2676:G:H8	1.79	0.47
1:X:2769:C:H2'	1:X:2770:A:C8	2.49	0.47
3:A:162:THR:OG1	3:A:197:VAL:HG22	2.15	0.47
3:A:247:PRO:C	3:A:249:THR:N	2.68	0.47
7:E:98:LEU:HD12	7:E:102:ALA:O	2.15	0.47
9:G:122:HIS:HB3	9:G:125:ARG:HG2	1.96	0.47
11:I:29:THR:O	11:I:30:ALA:CB	2.63	0.47
12:J:137:VAL:CG1	12:J:139:ASP:OD2	2.63	0.47
14:L:26:ARG:HD3	14:L:86:GLN:HB3	1.96	0.47
14:L:31:VAL:HG11	14:L:89:PHE:HE2	1.80	0.47
18:P:29:LYS:HB3	18:P:30:TYR:CD2	2.50	0.47
20:R:10:HIS:ND1	20:R:10:HIS:N	2.63	0.47
26:Z:16:ARG:NH1	26:Z:17:ASP:OD1	2.47	0.47
1:X:537:C:C5	1:X:2759:U:H2'	2.50	0.47
1:X:555:U:O2'	1:X:1234:C:H5'	2.14	0.47
2:Y:7:C:H2'	2:Y:8:C:H6	1.80	0.47
2:Y:58:G:C4'	2:Y:59:A:H8	2.28	0.47
2:Y:94:G:H5"	21:S:74:ARG:HH12	1.78	0.47
3:A:150:PRO:HD3	3:A:187:HIS:NE2	2.29	0.47
4:B:84:PHE:CD2	4:B:86:PRO:HD3	2.50	0.47
12:J:44:LYS:HB2	12:J:47:GLN:HG3	1.96	0.47
13:K:20:LEU:O	13:K:22:ARG:N	2.48	0.47
14:L:91:ARG:HB2	14:L:94:TYR:HD1	1.79	0.47
14:L:100:VAL:HG13	14:L:101:LYS:N	2.29	0.47
16:N:14:HIS:HD2	16:N:32:TYR:CE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:59:PHE:CD1	26:Z:30:LEU:CD1	2.97	0.47
18:P:66:GLU:O	18:P:69:ALA:HB3	2.15	0.47
20:R:81:VAL:HG11	20:R:89:GLY:HA2	1.97	0.47
21:S:1:MET:H1	21:S:52:PHE:HE2	1.63	0.47
1:X:591:G:C2'	1:X:592:G:H8	2.21	0.47
1:X:647:G:O2'	1:X:649:G:H4'	2.14	0.47
1:X:1025:A:C2	1:X:1160:C:C2	3.03	0.47
1:X:1438:G:H2'	1:X:1439:G:H5'	1.97	0.47
1:X:1496:G:H1'	1:X:1497:C:O5'	2.14	0.47
1:X:1725:C:C2	1:X:1742:G:N2	2.83	0.47
1:X:1978:U:H3'	1:X:1979:C:H5"	1.97	0.47
1:X:2407:G:H21	11:I:59:ARG:HH12	1.61	0.47
1:X:2705:A:H62	1:X:2707:G:N2	2.13	0.47
1:X:2793:G:O2'	1:X:2794:G:H5'	2.14	0.47
4:B:67:PHE:CE1	4:B:75:THR:HG22	2.50	0.47
5:C:22:VAL:HG21	5:C:110:SER:HA	1.97	0.47
7:E:103:LEU:HD12	7:E:104:GLU:N	2.30	0.47
10:H:70:VAL:O	10:H:70:VAL:HG13	2.15	0.47
11:I:14:LYS:HG3	11:I:14:LYS:O	2.15	0.47
11:I:55:ARG:O	11:I:56:LEU:HB2	2.15	0.47
12:J:76:THR:HA	12:J:89:GLY:O	2.15	0.47
14:L:31:VAL:HG11	14:L:89:PHE:CE2	2.50	0.47
15:M:34:ARG:HH21	15:M:91:VAL:CG2	2.23	0.47
16:N:22:LYS:C	16:N:24:PHE:H	2.19	0.47
1:X:31:C:O2'	1:X:32:C:H5'	2.15	0.47
1:X:115:G:C6	1:X:117:A:C6	3.03	0.47
1:X:393:U:O2'	23:U:18:VAL:HB	2.15	0.47
1:X:461:A:C5	1:X:462:G:C5	3.03	0.47
1:X:492:G:O2'	1:X:516:G:N2	2.48	0.47
1:X:1811:A:C4'	1:X:1812:U:O5'	2.58	0.47
1:X:1950:C:N4	1:X:1951:G:C6	2.83	0.47
1:X:2026:C:N3	1:X:2757:G:N2	2.63	0.47
1:X:2055:G:O2'	1:X:2056:C:H5'	2.15	0.47
1:X:2494:C:O2	1:X:2549:G:C2	2.68	0.47
1:X:2505:G:H1'	30:4:1:MET:HB3	1.97	0.47
1:X:2560:G:OP2	1:X:2560:G:N2	2.47	0.47
3:A:118:VAL:HG13	3:A:129:GLY:O	2.15	0.47
7:E:149:ARG:HA	7:E:162:VAL:HB	1.97	0.47
9:G:132:PHE:HB2	9:G:145:HIS:NE2	2.30	0.47
16:N:7:GLY:O	16:N:8:ILE:CG1	2.63	0.47
17:O:19:VAL:CG1	17:O:90:PHE:CD1	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:71:MET:N	21:S:71:MET:SD	2.88	0.47
1:X:165:G:H1	1:X:185:C:N4	2.04	0.46
1:X:306:G:H22	1:X:355:G:H1'	1.78	0.46
1:X:514:G:H2'	1:X:514:G:N3	2.30	0.46
1:X:538:A:O4'	1:X:539:A:OP1	2.33	0.46
1:X:618:A:C2	1:X:632:A:N7	2.82	0.46
1:X:638:A:N7	11:I:74:VAL:HG11	2.31	0.46
1:X:695:G:H5"	28:2:26:SER:CB	2.44	0.46
1:X:760:U:C4	26:Z:3:LYS:HG3	2.50	0.46
1:X:1950:C:C4	1:X:1951:G:C5	3.03	0.46
1:X:2256:G:P	12:J:86:LYS:HD2	2.55	0.46
1:X:2659:C:H2'	1:X:2660:C:C6	2.50	0.46
13:K:98:LEU:CD2	26:Z:56:GLN:HG2	2.41	0.46
16:N:86:ALA:C	16:N:88:ILE:N	2.69	0.46
1:X:654:A:N6	1:X:2348:A:O2'	2.48	0.46
1:X:1730:G:C2	1:X:1737:G:C2	3.02	0.46
1:X:1790:G:C5	3:A:178:LEU:HD13	2.50	0.46
1:X:2282:G:C2	1:X:2293:G:N2	2.82	0.46
1:X:2379:G:C2	1:X:2380:U:O2	2.68	0.46
1:X:2447:G:C8	1:X:2455:A:C2	3.03	0.46
31:X:2881:LMA:O55	31:X:2881:LMA:C34	2.64	0.46
5:C:163:ASN:HD22	5:C:164:VAL:N	2.13	0.46
9:G:104:THR:H	9:G:107:GLN:HG3	1.79	0.46
10:H:100:ASN:C	10:H:100:ASN:OD1	2.54	0.46
13:K:84:ALA:N	13:K:85:PRO:CD	2.78	0.46
19:Q:25:TYR:HE2	19:Q:82:LEU:HD12	1.80	0.46
20:R:84:VAL:HA	20:R:90:LYS:HE2	1.97	0.46
29:3:31:HIS:O	29:3:32:GLN:O	2.33	0.46
1:X:45:C:N4	1:X:191:G:OP2	2.48	0.46
1:X:48:A:N6	1:X:154:U:C5	2.81	0.46
1:X:491:A:H3'	1:X:492:G:H5"	1.97	0.46
1:X:591:G:H1	1:X:1271:C:N4	2.13	0.46
1:X:797:A:H5"	3:A:228:ASN:OD1	2.15	0.46
1:X:1312:G:H5"	1:X:1313:U:OP1	2.15	0.46
1:X:2240:C:C4	1:X:2259:G:N1	2.84	0.46
2:Y:89:G:C6	2:Y:93:G:C6	3.03	0.46
4:B:84:PHE:CZ	4:B:86:PRO:HG2	2.51	0.46
5:C:179:ASP:O	5:C:182:ARG:HB3	2.16	0.46
10:H:7:ARG:C	10:H:8:LEU:HD23	2.36	0.46
11:I:102:LYS:O	11:I:103:ASN:HB3	2.15	0.46
12:J:40:PRO:HB3	12:J:99:LYS:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:60:SER:CA	15:M:64:LYS:HB2	2.45	0.46
16:N:81:ASN:HD22	16:N:117:ARG:NH2	2.14	0.46
22:T:43:THR:CG2	22:T:46:LYS:HG2	2.45	0.46
1:X:42:G:H2'	1:X:43:A:O4'	2.16	0.46
1:X:170:U:H5"	1:X:816:U:H1'	1.97	0.46
1:X:476:G:H4'	28:2:16:HIS:ND1	2.31	0.46
1:X:633:G:H2'	1:X:634:G:H8	1.79	0.46
1:X:1514:C:H4'	1:X:1592:U:O2'	2.15	0.46
1:X:2371:A:O2'	11:I:59:ARG:O	2.23	0.46
7:E:157:TYR:O	7:E:171:LEU:HD23	2.15	0.46
9:G:141:GLY:O	9:G:144:MET:HB2	2.15	0.46
10:H:22:ILE:HB	10:H:52:VAL:HG12	1.97	0.46
10:H:47:VAL:HG22	10:H:77:THR:HG23	1.97	0.46
11:I:51:GLY:HA3	29:3:59:LYS:NZ	2.30	0.46
13:K:79:VAL:HA	13:K:83:VAL:CG2	2.45	0.46
16:N:13:ARG:O	16:N:17:VAL:HG23	2.16	0.46
17:O:22:VAL:HA	17:O:91:THR:HG22	1.96	0.46
25:W:12:ARG:HG2	25:W:12:ARG:HH11	1.81	0.46
1:X:82:G:N2	1:X:83:A:N6	2.60	0.46
1:X:303:C:H2'	1:X:304:A:H5"	1.98	0.46
1:X:317:U:C3'	1:X:318:G:H5'	2.46	0.46
1:X:518:A:N6	18:P:30:TYR:CE1	2.83	0.46
1:X:518:A:C6	18:P:30:TYR:CE1	3.04	0.46
1:X:742:G:N7	3:A:210:ALA:O	2.49	0.46
1:X:832:A:C4	1:X:1203:A:C2	3.04	0.46
1:X:1835:C:H5'	3:A:256:LYS:HE2	1.98	0.46
1:X:1840:A:H2'	1:X:1841:G:O4'	2.15	0.46
1:X:1981:A:H4'	1:X:2704:U:O2'	2.15	0.46
1:X:2522:G:H2'	1:X:2523:G:C8	2.50	0.46
1:X:2664:G:N2	1:X:2665:G:C1'	2.78	0.46
1:X:2819:G:H2'	1:X:2820:C:H6	1.79	0.46
3:A:135:ARG:HB3	3:A:188:SER:HB2	1.97	0.46
3:A:246:VAL:HG12	3:A:251:TRP:H	1.80	0.46
5:C:45:THR:HB	5:C:86:PRO:HG2	1.98	0.46
9:G:61:ARG:HE	9:G:65:LYS:HD2	1.78	0.46
28:2:15:THR:O	28:2:16:HIS:CB	2.61	0.46
1:X:2726:U:O5'	1:X:2726:U:H6	1.98	0.46
3:A:80:VAL:HB	3:A:115:GLY:N	2.21	0.46
4:B:44:TYR:HD1	4:B:82:ARG:NH1	2.14	0.46
4:B:61:LYS:HB3	4:B:62:PRO:HD3	1.97	0.46
4:B:120:TRP:O	4:B:121:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:103:LEU:HD12	7:E:104:GLU:H	1.81	0.46
9:G:132:PHE:CD2	9:G:145:HIS:HB2	2.51	0.46
15:M:55:ILE:HG22	15:M:104:LEU:HB2	1.98	0.46
1:X:178:C:H2'	1:X:179:U:C6	2.50	0.46
1:X:568:G:H2'	1:X:569:C:O4'	2.15	0.46
1:X:640:C:H4'	1:X:660:G:H21	1.81	0.46
1:X:1050:G:C2'	1:X:1051:U:H5'	2.45	0.46
1:X:1347:C:O2'	1:X:1348:C:H5'	2.16	0.46
1:X:1467:U:C3'	1:X:1467:U:C6	2.99	0.46
1:X:1469:U:H5'	1:X:1470:G:P	2.55	0.46
1:X:1496:G:H4'	1:X:1497:C:OP1	2.15	0.46
1:X:1672:A:O4'	4:B:113:THR:HG22	2.16	0.46
1:X:2026:C:C4	1:X:2757:G:N3	2.83	0.46
1:X:2327:U:H5'	27:1:21:TYR:CE1	2.50	0.46
1:X:2445:C:H2'	1:X:2446:C:C6	2.51	0.46
1:X:2677:U:H2'	1:X:2678:C:C6	2.51	0.46
1:X:2704:U:C2'	1:X:2705:A:C2	2.98	0.46
3:A:33:ALA:O	3:A:34:LEU:HB3	2.15	0.46
4:B:31:CYS:HB3	4:B:49:ILE:HG12	1.97	0.46
5:C:58:MET:HG2	5:C:59:TYR:N	2.31	0.46
10:H:2:ILE:HD12	10:H:2:ILE:HG23	1.69	0.46
10:H:7:ARG:O	10:H:8:LEU:HD23	2.16	0.46
15:M:6:LYS:N	15:M:6:LYS:HD2	2.31	0.46
15:M:24:LEU:HD11	15:M:34:ARG:HH22	1.81	0.46
15:M:82:PRO:O	15:M:84:ALA:N	2.48	0.46
18:P:37:LYS:HE2	18:P:64:ALA:H	1.80	0.46
1:X:513:A:C5	1:X:516:G:C6	3.04	0.46
1:X:699:G:H4'	1:X:700:C:OP2	2.15	0.46
1:X:820:U:H2'	1:X:821:A:C8	2.51	0.46
1:X:1141:U:N3	1:X:2008:C:H5"	2.30	0.46
1:X:1270:C:H4'	5:C:77:PHE:CD2	2.51	0.46
1:X:1326:U:O2	1:X:1326:U:H3'	2.16	0.46
1:X:1444:C:N4	1:X:1579:G:H1	2.08	0.46
1:X:1469:U:H5"	1:X:1470:G:C8	2.51	0.46
1:X:1628:C:H5'	28:2:7:PRO:CG	2.46	0.46
1:X:1641:C:H2'	1:X:1642:G:O4'	2.16	0.46
1:X:1712:G:C2'	1:X:1713:G:H5'	2.45	0.46
1:X:1790:G:C6	1:X:1811:A:N7	2.83	0.46
1:X:1841:G:C2'	1:X:1842:G:H5'	2.46	0.46
1:X:1854:G:H1'	1:X:1864:G:N2	2.31	0.46
1:X:2082:C:H2'	1:X:2083:G:H5'	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2442:C:H2'	1:X:2443:C:C6	2.51	0.46
1:X:2484:G:O2'	1:X:2485:U:C5'	2.61	0.46
1:X:2837:G:H2'	1:X:2838:U:C6	2.50	0.46
3:A:147:GLU:HB2	3:A:190:CYS:HB3	1.97	0.46
4:B:4:ILE:HD11	4:B:90:SER:O	2.16	0.46
12:J:86:LYS:O	12:J:88:LYS:HG3	2.16	0.46
13:K:20:LEU:HA	13:K:20:LEU:HD12	1.70	0.46
14:L:82:LYS:HB2	14:L:84:ILE:CD1	2.45	0.46
27:1:28:ARG:NH1	27:1:28:ARG:HB3	2.30	0.46
1:X:531:G:H2'	1:X:532:A:C8	2.50	0.46
1:X:579:G:OP1	1:X:983:G:O3'	2.34	0.46
1:X:1061:A:C2	1:X:2731:G:N1	2.84	0.46
1:X:1790:G:N2	3:A:156:LEU:HD23	2.31	0.46
1:X:1837:G:C2	1:X:1879:G:C2	3.04	0.46
1:X:1922:U:H3'	1:X:1923:U:H5"	1.98	0.46
1:X:2324:G:HO2'	1:X:2360:C:HO2'	1.46	0.46
1:X:2581:A:N3	1:X:2581:A:H5"	2.31	0.46
1:X:2736:U:OP2	30:4:17:VAL:HG11	2.16	0.46
3:A:118:VAL:HG22	3:A:129:GLY:HA3	1.97	0.46
4:B:16:LYS:HB3	4:B:21:ILE:HD11	1.97	0.46
9:G:84:ASN:O	9:G:85:ALA:HB3	2.16	0.46
10:H:116:ARG:O	10:H:116:ARG:CG	2.64	0.46
13:K:82:GLU:O	13:K:86:LYS:HG3	2.16	0.46
16:N:70:ARG:HG3	16:N:70:ARG:HH11	1.80	0.46
16:N:94:VAL:O	16:N:94:VAL:HG12	2.15	0.46
19:Q:34:THR:O	19:Q:38:ILE:HG22	2.16	0.46
19:Q:39:LYS:HA	19:Q:42:ILE:HG22	1.98	0.46
19:Q:58:VAL:HA	19:Q:59:PRO:HD2	1.61	0.46
1:X:168:A:H2'	1:X:169:C:H6	1.73	0.46
1:X:193:A:N3	1:X:445:A:C2	2.84	0.46
1:X:219:G:N2	1:X:232:A:OP2	2.45	0.46
1:X:242:A:N7	1:X:441:A:C6	2.84	0.46
1:X:314:G:C2	1:X:326:A:C2	3.04	0.46
1:X:321:A:P	20:R:27:GLY:H	2.40	0.46
1:X:689:A:C2	1:X:690:A:C8	3.04	0.46
1:X:1790:G:C6	3:A:178:LEU:HD13	2.50	0.46
1:X:1941:C:H2'	1:X:1942:G:H8	1.81	0.46
1:X:1947:G:O2'	1:X:1950:C:OP2	2.31	0.46
1:X:2014:A:C5	1:X:2477:C:H1'	2.51	0.46
1:X:2495:G:C2'	1:X:2496:C:H5'	2.45	0.46
1:X:2707:G:C8	1:X:2708:U:C5	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2862:G:H1'	26:Z:29:ASN:HD21	1.81	0.46
4:B:9:ILE:HD13	15:M:12:LEU:HD13	1.98	0.46
9:G:125:ARG:HD2	9:G:129:HIS:CE1	2.50	0.46
11:I:73:GLU:OE1	11:I:105:PRO:O	2.34	0.46
13:K:87:TYR:CE1	13:K:94:TYR:HB3	2.51	0.46
26:Z:51:TYR:CE2	26:Z:55:ARG:HB2	2.51	0.46
29:3:13:ARG:NH1	29:3:26:LYS:N	2.64	0.46
1:X:177:U:H4'	23:U:40:ARG:HE	1.81	0.45
1:X:812:G:H3'	1:X:813:A:H2'	1.97	0.45
1:X:825:C:H2'	1:X:826:U:H6	1.81	0.45
1:X:1289:A:C2	1:X:1290:A:C8	3.04	0.45
1:X:1573:G:O6	1:X:1574:A:N6	2.49	0.45
1:X:1790:G:H21	3:A:156:LEU:HD23	1.82	0.45
1:X:2048:C:O2'	1:X:2049:C:H5'	2.16	0.45
1:X:2477:C:H5'	1:X:2477:C:H6	1.81	0.45
1:X:2722:C:H2'	1:X:2723:C:C6	2.51	0.45
2:Y:72:C:H42	2:Y:109:G:H1	1.63	0.45
12:J:99:LYS:CD	12:J:100:PRO:HD2	2.45	0.45
15:M:9:ARG:HA	15:M:12:LEU:HD12	1.98	0.45
21:S:117:VAL:HG22	21:S:168:VAL:HA	1.98	0.45
25:W:40:VAL:HA	25:W:43:MET:HG3	1.98	0.45
27:1:18:THR:O	27:1:20:PHE:CE1	2.68	0.45
1:X:15:G:O2'	26:Z:18:MET:HA	2.15	0.45
1:X:15:G:C4'	26:Z:21:SER:HB2	2.45	0.45
1:X:321:A:OP1	20:R:26:SER:HA	2.15	0.45
1:X:333:A:C5	1:X:351:A:C2	3.05	0.45
1:X:696:U:H6	1:X:696:U:O5'	1.99	0.45
1:X:883:A:H1'	12:J:11:ARG:HH21	1.80	0.45
1:X:1022:A:OP1	16:N:75:ASN:ND2	2.50	0.45
1:X:1086:C:H3'	1:X:1087:C:C5'	2.36	0.45
1:X:1166:A:C5'	16:N:55:ARG:HH11	2.27	0.45
1:X:1226:A:N1	1:X:1250:A:H1'	2.31	0.45
1:X:1438:G:O2'	1:X:1439:G:H5'	2.16	0.45
1:X:1505:U:O2	1:X:1506:C:C5	2.68	0.45
1:X:1791:C:N4	1:X:1810:U:O2'	2.49	0.45
1:X:2245:A:H4'	1:X:2246:A:C4	2.50	0.45
1:X:2444:C:O2'	1:X:2445:C:H5'	2.16	0.45
1:X:2685:A:C2	1:X:2686:C:H1'	2.51	0.45
3:A:244:GLY:O	3:A:245:ARG:NE	2.49	0.45
5:C:39:ARG:HH21	5:C:91:TYR:CB	2.29	0.45
6:D:135:GLN:CD	6:D:150:ARG:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:28:GLY:O	10:H:35:THR:N	2.31	0.45
11:I:56:LEU:HD13	29:3:52:LYS:HE3	1.98	0.45
16:N:30:LYS:HB3	16:N:30:LYS:HZ2	1.81	0.45
26:Z:6:VAL:HG13	26:Z:7:PRO:CD	2.43	0.45
29:3:59:LYS:O	29:3:60:LEU:HB2	2.16	0.45
1:X:484:G:N1	1:X:485:G:C5	2.83	0.45
1:X:493:A:OP2	1:X:517:A:N6	2.42	0.45
1:X:538:A:C2	1:X:2025:A:C6	3.04	0.45
1:X:1631:C:H5	1:X:1633:C:C4	2.34	0.45
1:X:1643:A:H1'	1:X:1657:A:C2	2.50	0.45
1:X:1978:U:H2'	1:X:1979:C:H6	1.80	0.45
1:X:2218:G:O4'	3:A:250:PRO:HG3	2.15	0.45
3:A:90:SER:O	3:A:199:ASN:OD1	2.34	0.45
4:B:116:VAL:H	4:B:136:ARG:HE	1.65	0.45
9:G:70:PHE:CB	16:N:64:ARG:HG2	2.44	0.45
10:H:29:ILE:HB	10:H:34:LEU:HD23	1.97	0.45
11:I:35:LYS:O	11:I:36:GLY:O	2.34	0.45
12:J:26:ASP:HB3	12:J:27:TYR:H	1.61	0.45
13:K:35:GLN:HB3	13:K:112:LEU:HD23	1.98	0.45
14:L:37:HIS:CD2	14:L:39:TYR:CE1	3.05	0.45
14:L:42:ILE:HG22	14:L:53:ALA:N	2.31	0.45
18:P:79:ALA:HA	18:P:83:ASP:HB2	1.99	0.45
24:V:14:PHE:O	24:V:18:ILE:HG13	2.16	0.45
25:W:18:LYS:O	25:W:21:GLN:HB3	2.16	0.45
1:X:635:C:O2'	1:X:670:U:OP1	2.30	0.45
1:X:1414:G:C6	1:X:1415:C:N3	2.85	0.45
1:X:1756:C:O2'	1:X:1757:C:H5'	2.16	0.45
1:X:2265:A:H3'	27:1:32:GLN:HB2	1.97	0.45
1:X:2843:A:H2'	1:X:2844:G:O4'	2.15	0.45
3:A:246:VAL:HG12	3:A:252:GLY:H	1.78	0.45
8:F:75:SER:O	8:F:79:ARG:HG3	2.16	0.45
9:G:84:ASN:C	9:G:86:ALA:H	2.20	0.45
9:G:117:GLU:C	9:G:119:LEU:N	2.69	0.45
11:I:56:LEU:HB3	29:3:52:LYS:HZ1	1.81	0.45
14:L:67:THR:O	14:L:71:VAL:HG12	2.16	0.45
15:M:22:ARG:NH1	15:M:24:LEU:HD21	2.31	0.45
16:N:50:ARG:O	16:N:54:LYS:HE2	2.16	0.45
19:Q:91:LEU:HD22	19:Q:91:LEU:N	2.31	0.45
24:V:7:ARG:HD2	24:V:7:ARG:C	2.37	0.45
1:X:304:A:C5	1:X:359:G:N2	2.85	0.45
1:X:719:A:H2'	1:X:720:A:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:883:A:C5'	12:J:10:PHE:O	2.65	0.45
1:X:957:G:H2'	1:X:958:G:C8	2.51	0.45
1:X:1200:G:H2'	1:X:1201:G:O4'	2.17	0.45
1:X:1514:C:O4'	1:X:1593:C:H4'	2.16	0.45
1:X:1834:G:N2	1:X:1884:A:C5	2.85	0.45
1:X:1941:C:H2'	1:X:1942:G:C8	2.51	0.45
1:X:2087:U:H3	1:X:2169:A:H2	1.65	0.45
1:X:2201:G:H2'	1:X:2202:G:C8	2.51	0.45
1:X:2594:U:C6	26:Z:7:PRO:HA	2.52	0.45
4:B:116:VAL:CG1	4:B:136:ARG:HH21	2.29	0.45
19:Q:61:LYS:HG2	19:Q:61:LYS:O	2.15	0.45
1:X:207:U:O4	1:X:432:C:H4'	2.16	0.45
1:X:455:A:C2	1:X:1258:G:N3	2.83	0.45
1:X:495:C:H2'	1:X:496:C:C6	2.52	0.45
1:X:1174:G:C2	1:X:1175:A:C8	3.05	0.45
1:X:1437:A:H2'	1:X:1438:G:C8	2.52	0.45
1:X:1673:C:N4	1:X:1987:G:H1	2.15	0.45
1:X:1752:U:O5'	1:X:1752:U:H6	2.00	0.45
1:X:1791:C:P	3:A:264:ARG:HG3	2.56	0.45
1:X:1987:G:C5	1:X:1988:A:C8	3.04	0.45
1:X:2002:A:H62	26:Z:9:LYS:NZ	2.14	0.45
1:X:2708:U:H2'	1:X:2709:C:C6	2.52	0.45
9:G:55:ALA:HB1	9:G:134:MET:CE	2.46	0.45
11:I:49:PHE:CE1	29:3:59:LYS:HE3	2.51	0.45
11:I:53:ARG:HD2	11:I:53:ARG:C	2.37	0.45
20:R:60:PRO:HB2	20:R:61:SER:H	1.61	0.45
21:S:71:MET:HA	21:S:78:PRO:HA	1.98	0.45
25:W:14:GLY:O	25:W:18:LYS:HG2	2.17	0.45
1:X:27:G:N2	1:X:522:G:H1'	2.32	0.45
1:X:167:A:C4	1:X:184:A:C2	3.04	0.45
1:X:487:G:O4'	1:X:515:A:C2	2.70	0.45
1:X:537:C:H5	1:X:2759:U:H2'	1.82	0.45
1:X:686:C:O2'	1:X:687:G:H5'	2.17	0.45
1:X:854:G:H2'	1:X:855:G:C8	2.52	0.45
1:X:982:C:C4	1:X:983:G:N7	2.85	0.45
1:X:1226:A:C5	1:X:1250:A:N3	2.85	0.45
1:X:1332:G:C6	1:X:1333:G:C6	3.05	0.45
1:X:1763:G:C2'	1:X:1764:A:H5'	2.46	0.45
1:X:1770:U:O2	1:X:1774:A:C6	2.70	0.45
1:X:1805:G:N3	3:A:51:THR:HG21	2.31	0.45
1:X:2066:G:C6	1:X:2067:U:N3	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2299:A:H3'	1:X:2299:A:N3	2.31	0.45
5:C:72:ARG:HG3	5:C:77:PHE:CD2	2.51	0.45
6:D:61:THR:HG22	6:D:99:PHE:CD1	2.51	0.45
7:E:56:SER:H	7:E:61:HIS:CD2	2.35	0.45
11:I:45:LYS:C	11:I:45:LYS:HD3	2.37	0.45
11:I:107:LYS:HG3	11:I:108:LEU:N	2.32	0.45
12:J:71:PRO:HA	12:J:96:SER:HB2	1.99	0.45
14:L:11:LEU:HD23	14:L:14:ARG:NH1	2.31	0.45
18:P:40:LEU:HD22	26:Z:25:LEU:CD1	2.46	0.45
18:P:71:VAL:HG12	18:P:126:ILE:CG2	2.47	0.45
21:S:73:LYS:O	21:S:74:ARG:HB2	2.16	0.45
30:4:9:LYS:HD2	30:4:9:LYS:N	2.32	0.45
30:4:22:ARG:HD2	30:4:37:GLY:HA3	1.99	0.45
1:X:571:U:C4	1:X:2019:C:O4'	2.69	0.45
1:X:771:C:O2	1:X:1964:A:H2	1.99	0.45
1:X:1507:A:H5'	3:A:100:ASP:OD1	2.17	0.45
1:X:1710:U:H5'	1:X:1711:C:C5	2.51	0.45
1:X:2321:C:O2'	1:X:2353:G:H5"	2.17	0.45
1:X:2409:A:O2'	1:X:2410:U:C6	2.70	0.45
1:X:2551:A:C8	4:B:144:ARG:HD3	2.52	0.45
1:X:2651:U:H2'	1:X:2652:G:O5'	2.17	0.45
1:X:2702:G:H4'	13:K:5:LYS:HE2	1.99	0.45
2:Y:17:A:C1'	2:Y:112:A:C8	2.86	0.45
4:B:117:MET:HA	4:B:121:ASN:O	2.17	0.45
5:C:33:TRP:HD1	5:C:93:TYR:CE1	2.35	0.45
11:I:43:ALA:O	11:I:45:LYS:HB2	2.17	0.45
12:J:48:ILE:HD12	12:J:71:PRO:HG3	1.99	0.45
25:W:41:ARG:HB3	25:W:45:LYS:NZ	2.32	0.45
1:X:571:U:C2	1:X:581:A:C8	3.05	0.45
1:X:609:U:H4'	11:I:18:ARG:CZ	2.47	0.45
1:X:1017:C:H2'	1:X:1018:C:H6	1.82	0.45
1:X:1391:A:C4'	1:X:1392:U:OP1	2.64	0.45
1:X:1849:G:C6	1:X:1850:G:N1	2.85	0.45
1:X:2769:C:H1'	1:X:2866:A:H2	1.82	0.45
1:X:2780:A:O2'	1:X:2781:G:H5'	2.16	0.45
3:A:122:PRO:HG2	3:A:123:GLU:CD	2.38	0.45
6:D:34:ILE:HD13	6:D:156:ILE:HA	1.99	0.45
12:J:39:GLU:HB3	12:J:128:ILE:HB	1.99	0.45
15:M:99:VAL:CG2	15:M:100:ARG:N	2.79	0.45
16:N:66:ASN:OD1	16:N:66:ASN:N	2.47	0.45
23:U:67:LEU:HD23	23:U:67:LEU:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:124:A:OP2	28:2:44:VAL:HG11	2.17	0.45
1:X:757:U:H3	1:X:766:A:H61	1.65	0.45
1:X:832:A:N3	1:X:1203:A:C2	2.85	0.45
1:X:1008:G:O2'	1:X:1009:C:H5'	2.16	0.45
1:X:1381:G:H2'	1:X:1382:G:H8	1.82	0.45
1:X:1631:C:H5	1:X:1633:C:C5	2.34	0.45
1:X:1678:G:H4'	1:X:2691:C:N4	2.31	0.45
1:X:2260:C:C2'	1:X:2261:G:H5'	2.47	0.45
1:X:2825:A:C2	1:X:2826:C:C2	3.05	0.45
3:A:133:PRO:HD3	3:A:191:TYR:CE2	2.51	0.45
4:B:82:ARG:C	4:B:84:PHE:H	2.19	0.45
9:G:61:ARG:HE	9:G:65:LYS:HD3	1.80	0.45
9:G:116:ARG:HD2	9:G:119:LEU:HD12	1.99	0.45
9:G:154:GLU:OE2	9:G:155:THR:HG22	2.16	0.45
10:H:24:VAL:CG1	10:H:42:LYS:HG2	2.46	0.45
10:H:116:ARG:NE	15:M:38:LYS:HE3	2.32	0.45
16:N:106:PHE:O	16:N:110:VAL:HG23	2.17	0.45
19:Q:48:VAL:HG22	19:Q:49:ARG:O	2.16	0.45
20:R:25:LEU:HB2	20:R:81:VAL:HG23	1.98	0.45
1:X:648:A:H5"	11:I:110:ALA:O	2.17	0.44
1:X:830:C:O2'	1:X:852:U:H5"	2.17	0.44
1:X:940:G:O6	1:X:941:U:O4	2.35	0.44
1:X:1213:U:H2'	1:X:1214:C:C6	2.52	0.44
1:X:1283:C:H5"	1:X:1284:G:H5'	1.99	0.44
1:X:1405:A:N6	1:X:1406:A:N6	2.65	0.44
1:X:1710:U:H5'	1:X:1711:C:H5	1.82	0.44
1:X:1884:A:O2'	3:A:245:ARG:CG	2.64	0.44
1:X:2499:C:O2'	1:X:2500:C:H5'	2.17	0.44
1:X:2673:G:H2'	1:X:2674:C:H6	1.82	0.44
4:B:11:MET:HA	4:B:23:VAL:O	2.16	0.44
5:C:53:LYS:O	5:C:54:THR:OG1	2.30	0.44
5:C:163:ASN:HD22	5:C:163:ASN:C	2.21	0.44
12:J:29:ALA:HB3	12:J:68:ARG:NH2	2.30	0.44
12:J:36:ILE:CG2	12:J:37:ALA:N	2.80	0.44
18:P:118:LYS:HE3	18:P:118:LYS:HB2	1.80	0.44
29:3:13:ARG:HD3	29:3:25:PHE:HD1	1.83	0.44
1:X:430:C:H1'	1:X:2386:G:N2	2.32	0.44
1:X:627:A:H2'	1:X:628:A:C8	2.52	0.44
1:X:641:G:H4'	1:X:651:C:O2'	2.18	0.44
1:X:693:A:C5	1:X:811:G:N2	2.85	0.44
1:X:820:U:H2'	1:X:821:A:H8	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:867:G:H1	1:X:935:C:H42	1.65	0.44
1:X:918:A:C2'	1:X:919:U:H5"	2.40	0.44
1:X:1656:U:H4'	1:X:2678:C:H4'	1.99	0.44
1:X:1674:C:O2	1:X:1674:C:C2'	2.64	0.44
1:X:2340:C:P	29:3:27:SER:OG	2.75	0.44
1:X:2494:C:H2'	1:X:2495:G:C8	2.52	0.44
1:X:2825:A:C6	1:X:2826:C:C4	3.05	0.44
4:B:14:ILE:HD12	4:B:23:VAL:CG2	2.43	0.44
9:G:66:HIS:O	9:G:70:PHE:CE1	2.70	0.44
11:I:120:VAL:HB	11:I:140:VAL:HG22	1.98	0.44
15:M:31:ASP:HA	15:M:52:GLY:O	2.18	0.44
17:O:36:LYS:HE2	17:O:56:VAL:HG13	1.99	0.44
22:T:12:ASN:C	22:T:14:ARG:H	2.20	0.44
1:X:43:A:C6	1:X:44:G:C6	3.05	0.44
1:X:459:A:N6	1:X:484:G:C4	2.85	0.44
1:X:538:A:H62	1:X:2026:C:C5'	2.30	0.44
1:X:546:A:H2'	1:X:547:U:C6	2.53	0.44
1:X:822:G:H2'	1:X:823:U:H5'	1.99	0.44
1:X:1567:A:H2'	1:X:1568:A:O4'	2.16	0.44
1:X:1923:U:H4'	1:X:1924:C:O5'	2.17	0.44
1:X:1924:C:C2	1:X:1948:C:C2	3.05	0.44
1:X:2173:G:H2'	1:X:2174:G:C8	2.52	0.44
1:X:2200:G:O2'	3:A:150:PRO:HG2	2.17	0.44
3:A:56:GLY:H	3:A:218:ARG:H	1.65	0.44
4:B:32:PRO:HD2	4:B:50:GLY:O	2.16	0.44
9:G:162:LYS:H	9:G:163:PRO:CD	2.20	0.44
13:K:71:HIS:N	13:K:71:HIS:HD1	2.15	0.44
15:M:104:LEU:HA	15:M:106:TYR:CD2	2.51	0.44
18:P:19:LYS:O	18:P:20:LEU:CB	2.66	0.44
20:R:6:ALA:C	20:R:8:SER:H	2.21	0.44
20:R:51:VAL:O	20:R:51:VAL:HG12	2.17	0.44
1:X:1437:A:C2	1:X:1592:U:O2	2.70	0.44
1:X:1453:A:C2	1:X:1569:A:C6	3.06	0.44
1:X:1722:G:C6	1:X:1723:U:N3	2.86	0.44
1:X:2754:C:H2'	1:X:2755:A:O4'	2.17	0.44
2:Y:47:A:C8	6:D:92:ARG:NH1	2.85	0.44
5:C:3:GLN:HB2	5:C:116:LYS:HD2	1.99	0.44
6:D:29:PRO:HB2	6:D:169:LEU:HD22	2.00	0.44
6:D:78:LYS:HG2	6:D:80:ARG:NH1	2.32	0.44
10:H:60:PRO:O	10:H:61:ARG:HB2	2.17	0.44
12:J:22:ALA:HA	12:J:99:LYS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:99:LYS:HG3	12:J:100:PRO:HD2	2.00	0.44
22:T:45:PHE:CD2	22:T:77:ARG:HB3	2.52	0.44
1:X:395:G:C2	1:X:406:G:C2	3.05	0.44
1:X:637:G:H1	11:I:101:ARG:CD	2.30	0.44
1:X:779:U:O4	1:X:780:U:O4	2.36	0.44
1:X:819:C:H2'	1:X:820:U:C6	2.53	0.44
1:X:1450:G:N3	1:X:1573:G:C2	2.85	0.44
1:X:2494:C:C2	1:X:2549:G:C2	3.06	0.44
1:X:2495:G:C6	1:X:2496:C:N4	2.86	0.44
1:X:2616:U:H5"	4:B:82:ARG:HH22	1.80	0.44
3:A:47:ARG:HD3	3:A:47:ARG:C	2.38	0.44
3:A:69:LYS:H	3:A:69:LYS:CD	2.23	0.44
3:A:71:ARG:HH12	3:A:150:PRO:CB	2.30	0.44
9:G:93:LYS:HB3	9:G:97:ASP:HB3	1.99	0.44
9:G:132:PHE:CB	9:G:145:HIS:CD2	2.99	0.44
13:K:12:ARG:NH2	13:K:20:LEU:HD22	2.32	0.44
19:Q:53:ILE:CD1	19:Q:80:VAL:HG12	2.42	0.44
21:S:107:GLU:HA	21:S:111:GLY:O	2.17	0.44
28:2:41:GLN:OE1	28:2:41:GLN:HA	2.17	0.44
1:X:538:A:N3	1:X:538:A:C2'	2.79	0.44
1:X:576:A:O3'	11:I:40:ARG:NH1	2.51	0.44
1:X:843:G:O4'	1:X:2427:A:N1	2.51	0.44
1:X:861:G:N2	1:X:943:U:H1'	2.33	0.44
1:X:1817:U:H4'	3:A:253:LYS:HZ2	1.82	0.44
1:X:2235:G:N2	1:X:2254:C:C4	2.86	0.44
1:X:2670:C:O3'	1:X:2846:G:H4'	2.18	0.44
3:A:151:GLY:O	3:A:153:GLY:N	2.51	0.44
5:C:191:ALA:HA	5:C:194:GLU:HB3	1.99	0.44
7:E:105:MET:CE	7:E:131:ILE:HD11	2.47	0.44
11:I:43:ALA:O	11:I:44:GLY:C	2.55	0.44
1:X:13:A:C2	1:X:15:G:C6	3.06	0.44
1:X:155:G:O2'	1:X:156:G:H5'	2.17	0.44
1:X:459:A:C2	1:X:466:A:H2'	2.52	0.44
1:X:538:A:H4'	9:G:139:ARG:NE	2.33	0.44
1:X:541:C:N3	1:X:572:G:C8	2.86	0.44
1:X:935:C:C1'	22:T:29:GLU:HG2	2.46	0.44
1:X:1001:A:H1'	1:X:1167:A:C2	2.53	0.44
1:X:1422:C:H2'	1:X:1423:A:C8	2.53	0.44
1:X:1692:C:H2'	1:X:1693:A:O4'	2.18	0.44
1:X:2245:A:H5'	1:X:2246:A:C4	2.53	0.44
1:X:2329:C:H3'	1:X:2329:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2490:U:H2'	1:X:2491:C:C6	2.52	0.44
1:X:2554:C:O2'	4:B:140:SER:CB	2.66	0.44
1:X:2780:A:H2'	1:X:2781:G:C8	2.53	0.44
4:B:14:ILE:HG12	15:M:20:HIS:HD2	1.76	0.44
11:I:107:LYS:HE2	11:I:107:LYS:HB2	1.84	0.44
14:L:37:HIS:HE1	14:L:57:ALA:HB2	1.76	0.44
23:U:59:THR:O	23:U:60:VAL:C	2.56	0.44
29:3:36:LYS:HB2	29:3:36:LYS:HE2	1.83	0.44
1:X:317:U:O2'	1:X:1224:A:N7	2.50	0.44
1:X:409:G:O3'	23:U:47:HIS:CE1	2.71	0.44
1:X:813:A:O4'	1:X:815:A:H5'	2.17	0.44
1:X:1007:A:C5	1:X:1171:A:C2	3.06	0.44
1:X:1070:G:H5'	1:X:1071:U:H2'	1.99	0.44
1:X:1255:A:C6	1:X:1256:C:C4	3.06	0.44
1:X:2026:C:H2'	1:X:2027:C:H6	1.82	0.44
1:X:2289:A:N3	6:D:79:LEU:HD21	2.33	0.44
1:X:2436:U:O2'	1:X:2437:G:H5'	2.18	0.44
1:X:2659:C:H2'	1:X:2660:C:H6	1.82	0.44
4:B:67:PHE:CD2	4:B:74:PRO:HA	2.53	0.44
5:C:38:ARG:NH2	5:C:178:TYR:CE2	2.84	0.44
14:L:72:GLY:O	14:L:75:LEU:HB3	2.18	0.44
14:L:99:ARG:HG3	14:L:100:VAL:H	1.82	0.44
1:X:313:U:O2'	1:X:314:G:H5'	2.18	0.44
1:X:555:U:HO2'	1:X:556:A:P	2.41	0.44
1:X:688:A:H5'	5:C:61:GLN:OE1	2.18	0.44
1:X:768:U:C4	1:X:769:C:C4	3.05	0.44
1:X:815:A:C6	1:X:816:U:N3	2.86	0.44
1:X:913:A:N7	1:X:914:C:C4	2.86	0.44
1:X:987:G:C2	1:X:988:G:C8	3.05	0.44
1:X:1173:G:H2'	1:X:1174:G:C8	2.52	0.44
1:X:1313:U:H4'	1:X:1314:A:H5"	2.00	0.44
1:X:1335:A:C2	1:X:1346:C:O2'	2.69	0.44
1:X:1361:G:C6	1:X:1362:A:C6	3.06	0.44
1:X:1506:C:H2'	1:X:1507:A:H5'	1.99	0.44
1:X:1974:U:C2'	1:X:1975:G:C5'	2.96	0.44
1:X:2057:U:C2	1:X:2415:G:N2	2.86	0.44
1:X:2821:G:H2'	1:X:2822:U:O4'	2.18	0.44
3:A:89:ARG:O	3:A:90:SER:C	2.55	0.44
5:C:102:LEU:HD23	5:C:102:LEU:C	2.37	0.44
6:D:51:ASP:HA	6:D:54:ALA:HB3	1.99	0.44
9:G:55:ALA:HB1	9:G:134:MET:HE1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:111:LYS:HG3	9:G:111:LYS:O	2.17	0.44
10:H:114:VAL:O	10:H:115:ALA:O	2.36	0.44
20:R:16:PHE:HZ	20:R:46:VAL:CG2	2.31	0.44
21:S:127:PRO:C	21:S:129:ARG:H	2.21	0.44
22:T:18:PRO:O	22:T:19:LYS:HG2	2.17	0.44
1:X:122:G:H2'	28:2:19:ARG:NH2	2.33	0.43
1:X:538:A:N3	1:X:2025:A:C6	2.86	0.43
1:X:542:A:OP1	1:X:570:G:N2	2.49	0.43
1:X:599:A:H61	1:X:679:C:N4	2.16	0.43
1:X:1026:U:O2'	1:X:1027:C:H5'	2.18	0.43
1:X:1356:G:H8	1:X:1356:G:O5'	2.01	0.43
1:X:1686:A:OP2	1:X:1687:C:H5	2.01	0.43
1:X:1812:U:O2	3:A:160:ALA:O	2.34	0.43
1:X:1922:U:OP1	1:X:2583:U:O2'	2.32	0.43
1:X:2210:C:C4	1:X:2211:U:C4	3.06	0.43
1:X:2285:U:O2	6:D:44:LYS:HD2	2.18	0.43
1:X:2668:U:O2	1:X:2693:U:O4'	2.36	0.43
1:X:2700:U:O2	1:X:2700:U:C2'	2.64	0.43
2:Y:8:C:O2'	14:L:39:TYR:CE1	2.70	0.43
3:A:245:ARG:HD3	3:A:245:ARG:N	2.33	0.43
4:B:176:ARG:HH21	15:M:16:ILE:HA	1.83	0.43
5:C:54:THR:HB	5:C:73:SER:HB3	1.99	0.43
5:C:111:ARG:HH12	5:C:181:LEU:HD12	1.82	0.43
10:H:22:ILE:HD13	10:H:22:ILE:HG21	1.76	0.43
12:J:70:PHE:HA	12:J:71:PRO:HD3	1.66	0.43
13:K:20:LEU:O	13:K:21:ALA:C	2.55	0.43
23:U:22:GLY:HA3	23:U:39:LYS:CE	2.46	0.43
1:X:620:G:N2	1:X:630:G:H1'	2.32	0.43
1:X:869:C:H4'	22:T:69:PHE:HB2	1.98	0.43
1:X:1223:G:H5'	1:X:1225:G:O4'	2.18	0.43
1:X:1223:G:H4'	1:X:1224:A:C5'	2.48	0.43
1:X:1223:G:C5	1:X:1250:A:N6	2.86	0.43
1:X:1381:G:H2'	1:X:1382:G:C8	2.53	0.43
1:X:1405:A:C6	1:X:1406:A:C6	3.05	0.43
1:X:1511:A:N6	1:X:1512:A:N6	2.66	0.43
1:X:1631:C:C5	1:X:1633:C:C2	3.06	0.43
1:X:1724:C:C4	1:X:1747:G:C6	3.05	0.43
1:X:1835:C:C5'	3:A:256:LYS:HE2	2.48	0.43
1:X:1838:G:N2	1:X:1878:C:C2	2.86	0.43
1:X:1991:C:H2'	1:X:1992:G:C8	2.46	0.43
1:X:2053:G:C2	1:X:2421:C:C2	3.05	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2065:A:C2	1:X:2218:G:N3	2.86	0.43
1:X:2705:A:N7	1:X:2707:G:C5	2.85	0.43
1:X:2815:C:N4	1:X:2852:G:H1	2.16	0.43
3:A:69:LYS:HD3	3:A:69:LYS:N	2.25	0.43
3:A:207:LEU:C	3:A:212:ARG:HD3	2.38	0.43
10:H:82:LYS:HB2	10:H:82:LYS:HE3	1.78	0.43
1:X:475:U:C2	1:X:801:A:C6	3.06	0.43
1:X:799:C:O2'	1:X:800:U:H5'	2.19	0.43
1:X:1336:G:C2	1:X:1346:C:H1'	2.53	0.43
1:X:1342:U:H3'	1:X:1343:C:H6	1.82	0.43
1:X:1346:C:H6	1:X:1346:C:O5'	2.02	0.43
1:X:2043:A:N6	5:C:68:ARG:HH12	2.16	0.43
1:X:2062:U:H2'	1:X:2063:A:C8	2.54	0.43
1:X:2664:G:H2'	1:X:2664:G:N3	2.32	0.43
2:Y:12:C:H2'	2:Y:13:C:O4'	2.18	0.43
3:A:106:ILE:HG22	3:A:107:LEU:N	2.34	0.43
3:A:214:ARG:HD2	3:A:214:ARG:HA	1.84	0.43
4:B:54:LYS:HD2	4:B:59:VAL:HG22	1.99	0.43
7:E:105:MET:HE2	7:E:105:MET:HA	2.01	0.43
9:G:30:LYS:HB2	9:G:30:LYS:HE3	1.68	0.43
16:N:86:ALA:C	16:N:88:ILE:H	2.21	0.43
17:O:48:GLY:O	17:O:49:GLU:HB2	2.19	0.43
23:U:49:LYS:HB3	23:U:61:TRP:CD2	2.53	0.43
26:Z:42:SER:O	26:Z:44:HIS:CD2	2.55	0.43
1:X:320:A:H1'	1:X:340:G:N3	2.34	0.43
1:X:1252:C:H3'	1:X:1252:C:H6	1.83	0.43
1:X:1441:A:O4'	1:X:1442:C:C5	2.71	0.43
1:X:2445:C:C4	1:X:2446:C:N4	2.86	0.43
3:A:27:LYS:HE2	3:A:205:ILE:HD13	2.01	0.43
3:A:148:LEU:HD21	3:A:156:LEU:HD11	1.98	0.43
3:A:247:PRO:HD3	3:A:253:LYS:CG	2.49	0.43
7:E:56:SER:HB2	7:E:61:HIS:CE1	2.54	0.43
9:G:33:ILE:HB	9:G:34:PRO:HD2	2.01	0.43
17:O:29:ALA:HA	17:O:59:GLU:HB3	1.99	0.43
18:P:30:TYR:H	18:P:123:HIS:CE1	2.36	0.43
19:Q:35:LYS:HA	19:Q:38:ILE:HG22	1.98	0.43
22:T:32:LYS:H	22:T:35:ASN:HD22	1.65	0.43
24:V:6:MET:HE3	24:V:56:VAL:HG21	2.01	0.43
24:V:56:VAL:O	24:V:59:GLU:HB2	2.18	0.43
30:4:24:LEU:HD23	30:4:35:ARG:CZ	2.49	0.43
1:X:470:U:OP1	28:2:40:HIS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:608:G:H2'	1:X:609:U:C6	2.53	0.43
1:X:684:C:C5	11:I:43:ALA:HA	2.53	0.43
1:X:797:A:O2'	1:X:798:G:H8	2.02	0.43
1:X:1002:C:O2	1:X:1175:A:C2	2.72	0.43
1:X:1220:G:N2	1:X:1253:C:C4	2.86	0.43
1:X:1467:U:H3'	1:X:1467:U:C6	2.53	0.43
1:X:1673:C:O2'	1:X:1674:C:H5'	2.18	0.43
1:X:2064:U:O2'	1:X:2065:A:H5'	2.18	0.43
1:X:2300:G:H3'	1:X:2300:G:N3	2.34	0.43
1:X:2370:G:H2'	1:X:2371:A:H2	1.83	0.43
1:X:2565:C:O2	1:X:2565:C:H2'	2.18	0.43
3:A:46:ASN:O	3:A:47:ARG:C	2.55	0.43
7:E:137:ASP:O	7:E:141:VAL:HG23	2.18	0.43
10:H:23:ARG:HB3	10:H:23:ARG:CZ	2.48	0.43
12:J:36:ILE:HG22	12:J:37:ALA:N	2.33	0.43
16:N:29:SER:C	16:N:30:LYS:HG2	2.38	0.43
19:Q:10:PRO:HD3	24:V:30:PHE:HD2	1.83	0.43
1:X:66:U:H1'	1:X:87:G:N2	2.33	0.43
1:X:635:C:C3'	1:X:636:G:H5"	2.49	0.43
1:X:854:G:H1	1:X:948:C:N4	2.12	0.43
1:X:916:U:C4	1:X:917:U:C4	3.07	0.43
1:X:957:G:H2'	1:X:958:G:H8	1.84	0.43
1:X:1411:C:H2'	1:X:1412:C:H5'	2.00	0.43
1:X:1810:U:H5	3:A:158:ARG:NH1	2.16	0.43
1:X:1965:U:H2'	1:X:1966:C:H6	1.83	0.43
3:A:185:ARG:HH21	3:A:269:ARG:HH11	1.66	0.43
4:B:59:VAL:HG12	4:B:64:GLN:HG3	1.99	0.43
9:G:156:HIS:N	9:G:157:PRO:CD	2.82	0.43
12:J:21:ASP:C	12:J:99:LYS:HG2	2.38	0.43
18:P:14:ARG:HA	18:P:17:GLN:CG	2.48	0.43
24:V:17:GLU:O	24:V:21:ARG:HD3	2.18	0.43
1:X:64:C:H3'	1:X:64:C:H6	1.82	0.43
1:X:227:G:C6	1:X:228:A:C6	3.07	0.43
1:X:1817:U:C4'	3:A:253:LYS:HD2	2.49	0.43
1:X:2426:G:C2'	1:X:2479:U:OP2	2.66	0.43
1:X:2742:G:O2'	1:X:2743:G:H5'	2.18	0.43
1:X:2766:U:O2'	1:X:2767:C:H5'	2.19	0.43
1:X:2791:C:C2	1:X:2806:G:N2	2.86	0.43
4:B:14:ILE:CG1	15:M:20:HIS:CD2	2.88	0.43
6:D:77:PHE:HB3	6:D:78:LYS:H	1.58	0.43
8:F:74:MET:SD	8:F:127:VAL:HG22	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:103:TYR:CE1	9:G:111:LYS:C	2.92	0.43
11:I:52:GLY:O	11:I:53:ARG:HB3	2.19	0.43
13:K:79:VAL:HG13	13:K:80:MET:H	1.83	0.43
14:L:33:ARG:NH2	14:L:103:LEU:HD12	2.34	0.43
16:N:20:ARG:HD2	16:N:39:LEU:HD13	2.01	0.43
19:Q:48:VAL:HG21	19:Q:82:LEU:HD22	2.00	0.43
1:X:83:A:H1'	1:X:84:G:O4'	2.18	0.43
1:X:618:A:OP1	5:C:94:THR:HG21	2.19	0.43
1:X:637:G:H1	11:I:101:ARG:CG	2.32	0.43
1:X:1439:G:C2	1:X:1440:G:C2	3.07	0.43
1:X:2391:A:C8	1:X:2392:G:C8	3.07	0.43
1:X:2696:A:H2'	1:X:2697:G:C8	2.52	0.43
9:G:156:HIS:HB2	9:G:157:PRO:HD3	2.01	0.43
10:H:104:GLU:HG2	10:H:125:LYS:NZ	2.33	0.43
15:M:46:ARG:HG2	15:M:47:SER:N	2.34	0.43
15:M:103:LYS:O	15:M:104:LEU:CB	2.65	0.43
18:P:107:ILE:O	18:P:107:ILE:HG23	2.18	0.43
29:3:13:ARG:C	29:3:23:MET:O	2.56	0.43
1:X:239:A:H5'	1:X:620:G:O2'	2.18	0.43
1:X:321:A:OP1	20:R:27:GLY:N	2.47	0.43
1:X:482:A:N6	1:X:483:A:C2	2.87	0.43
1:X:538:A:H3'	9:G:142:ARG:NH1	2.30	0.43
1:X:872:G:OP2	1:X:872:G:C8	2.72	0.43
1:X:1047:G:N2	1:X:1131:G:C4	2.87	0.43
1:X:1069:G:C3'	1:X:1070:G:H5"	2.49	0.43
1:X:1356:G:N2	1:X:1418:C:N3	2.67	0.43
1:X:1673:C:H5'	4:B:136:ARG:HD3	2.01	0.43
5:C:163:ASN:ND2	5:C:163:ASN:C	2.72	0.43
9:G:61:ARG:HH22	9:G:78:ASP:HB2	1.84	0.43
10:H:116:ARG:NH1	15:M:38:LYS:HE3	2.33	0.43
20:R:77:HIS:C	20:R:79:SER:H	2.22	0.43
21:S:88:TYR:O	21:S:127:PRO:HG2	2.19	0.43
21:S:137:ASP:OD2	21:S:138:VAL:N	2.52	0.43
22:T:41:ARG:HD3	22:T:41:ARG:HA	1.76	0.43
23:U:32:ARG:HB2	23:U:33:LYS:H	1.63	0.43
28:2:14:LYS:O	28:2:14:LYS:HD3	2.19	0.43
1:X:940:G:C6	1:X:941:U:C4	3.07	0.43
1:X:1166:A:C2'	1:X:1167:A:H5"	2.49	0.43
1:X:1226:A:C4	1:X:1250:A:N3	2.87	0.43
1:X:1313:U:H4'	1:X:1314:A:O5'	2.18	0.43
1:X:1345:G:C5	1:X:1625:A:C5	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1779:C:C5	1:X:1780:A:N7	2.87	0.43
1:X:2238:G:C5	1:X:2406:C:N4	2.87	0.43
1:X:2323:U:O2'	27:1:40:TYR:CE1	2.71	0.43
1:X:2594:U:H2'	1:X:2595:C:H6	1.83	0.43
2:Y:5:C:H2'	2:Y:6:C:O4'	2.19	0.43
3:A:262:ARG:O	3:A:265:LYS:HB3	2.19	0.43
6:D:12:VAL:O	6:D:16:LEU:HG	2.19	0.43
13:K:5:LYS:HE2	13:K:5:LYS:HB2	1.78	0.43
18:P:16:GLN:H	18:P:16:GLN:HG2	1.70	0.43
1:X:43:A:H2	1:X:448:C:H41	1.65	0.42
1:X:196:A:O2'	1:X:197:G:H5'	2.19	0.42
1:X:314:G:C6	1:X:326:A:C2	3.06	0.42
1:X:396:U:C4	1:X:398:C:C5	3.07	0.42
1:X:701:U:O5'	1:X:701:U:H6	2.01	0.42
1:X:840:U:C5	1:X:2409:A:C5	3.07	0.42
1:X:922:A:N7	1:X:923:A:C6	2.86	0.42
1:X:943:U:O2'	1:X:944:A:O4'	2.34	0.42
1:X:1166:A:H2'	1:X:1167:A:H5"	2.01	0.42
1:X:1453:A:C8	1:X:1454:U:C6	3.07	0.42
1:X:2301:A:H2'	1:X:2302:G:O4'	2.19	0.42
4:B:38:THR:HG22	4:B:40:GLN:H	1.84	0.42
5:C:148:VAL:HG12	5:C:149:LEU:N	2.34	0.42
10:H:116:ARG:HD2	15:M:38:LYS:CE	2.49	0.42
11:I:77:LEU:HB3	11:I:112:GLY:H	1.84	0.42
18:P:29:LYS:O	18:P:30:TYR:HB2	2.19	0.42
18:P:31:VAL:O	18:P:33:MET:N	2.43	0.42
23:U:22:GLY:HA3	23:U:39:LYS:CD	2.49	0.42
29:3:13:ARG:HD2	29:3:25:PHE:CD1	2.54	0.42
1:X:7:G:H2'	1:X:8:A:O4'	2.19	0.42
1:X:334:G:N2	5:C:162:ARG:HH22	2.17	0.42
1:X:531:G:O2'	1:X:532:A:H5'	2.19	0.42
1:X:637:G:H8	1:X:637:G:O5'	2.02	0.42
1:X:1407:G:O6	1:X:1408:A:N6	2.52	0.42
1:X:1462:C:H2'	1:X:1463:A:C8	2.54	0.42
1:X:1508:G:H5'	1:X:1509:A:H5"	2.00	0.42
1:X:1836:C:N3	1:X:1880:G:N2	2.67	0.42
1:X:2053:G:C2	1:X:2054:A:N3	2.88	0.42
1:X:2293:G:C5'	6:D:35:VAL:HG11	2.45	0.42
1:X:2327:U:O5'	1:X:2327:U:H6	2.02	0.42
1:X:2363:G:OP1	22:T:55:ARG:HD2	2.19	0.42
1:X:2407:G:N2	11:I:59:ARG:HH22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2697:G:H2'	1:X:2698:G:O4'	2.20	0.42
1:X:2705:A:H4'	1:X:2706:U:OP1	2.18	0.42
2:Y:93:G:OP1	12:J:19:THR:HB	2.19	0.42
3:A:91:ALA:HA	3:A:199:ASN:OD1	2.19	0.42
5:C:172:VAL:O	5:C:172:VAL:HG12	2.19	0.42
7:E:55:PRO:HB2	7:E:61:HIS:CD2	2.54	0.42
9:G:61:ARG:CD	9:G:65:LYS:HD2	2.49	0.42
13:K:73:LYS:O	13:K:76:VAL:CG1	2.67	0.42
14:L:40:ALA:HB2	14:L:103:LEU:HD11	2.01	0.42
14:L:42:ILE:HD13	14:L:42:ILE:C	2.39	0.42
18:P:25:PHE:HD1	18:P:127:ILE:CD1	2.28	0.42
18:P:117:ILE:HG23	18:P:117:ILE:HD12	1.72	0.42
24:V:6:MET:HE2	24:V:56:VAL:HG21	2.02	0.42
1:X:68:C:H2'	1:X:69:G:O4'	2.19	0.42
1:X:331:U:H1'	5:C:162:ARG:HH21	1.84	0.42
1:X:700:C:O4'	28:2:4:THR:HA	2.18	0.42
1:X:971:A:H5"	1:X:972:C:OP2	2.19	0.42
1:X:1058:G:H2'	1:X:1121:G:O6	2.19	0.42
1:X:1615:C:OP1	19:Q:35:LYS:HB2	2.20	0.42
1:X:1685:A:C4	1:X:1691:G:N7	2.87	0.42
1:X:2045:A:C6	31:X:2881:LMA:H27	2.54	0.42
1:X:2497:A:N3	1:X:2497:A:H2'	2.34	0.42
1:X:2594:U:C2	26:Z:7:PRO:HA	2.54	0.42
5:C:3:GLN:O	5:C:12:GLY:HA3	2.18	0.42
6:D:112:ARG:H	6:D:112:ARG:CD	2.30	0.42
10:H:27:SER:HB3	10:H:50:ILE:H	1.82	0.42
10:H:116:ARG:HH22	15:M:41:GLU:HG2	1.83	0.42
12:J:78:LYS:HE2	12:J:81:GLU:HA	2.01	0.42
13:K:100:VAL:HG12	13:K:101:GLY:H	1.75	0.42
18:P:47:GLY:HA2	18:P:92:VAL:O	2.19	0.42
28:2:34:ARG:HH11	28:2:42:LEU:CA	2.32	0.42
1:X:318:G:N1	1:X:321:A:OP2	2.52	0.42
1:X:341:A:H2	1:X:1223:G:C8	2.37	0.42
1:X:404:A:C2	1:X:424:G:C2	3.08	0.42
1:X:487:G:H4'	1:X:512:A:H61	1.84	0.42
1:X:604:U:H5"	29:3:61:MET:SD	2.59	0.42
1:X:860:U:O2	1:X:860:U:H2'	2.17	0.42
1:X:1279:G:O2'	1:X:1995:G:O6	2.23	0.42
1:X:1326:U:O2	1:X:1326:U:C2'	2.65	0.42
1:X:1363:C:O2'	1:X:1364:C:H5'	2.20	0.42
1:X:1672:A:O4'	4:B:113:THR:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1710:U:H4'	1:X:1711:C:OP2	2.20	0.42
1:X:2740:C:O2'	1:X:2741:G:H5'	2.19	0.42
9:G:140:GLN:O	9:G:144:MET:HG3	2.19	0.42
23:U:50:ALA:HB1	23:U:52:ARG:NH2	2.33	0.42
1:X:5:A:O2'	1:X:6:A:H5'	2.19	0.42
1:X:357:A:H2'	1:X:358:C:H5'	2.02	0.42
1:X:413:G:O2'	1:X:414:A:H5"	2.19	0.42
1:X:421:G:O2'	1:X:422:C:H5'	2.19	0.42
1:X:470:U:O4	1:X:481:A:C8	2.72	0.42
1:X:623:G:C3'	1:X:624:A:H5"	2.50	0.42
1:X:688:A:H4'	5:C:61:GLN:CG	2.49	0.42
1:X:781:G:H2'	1:X:782:U:O4'	2.19	0.42
1:X:805:G:C5	1:X:2419:C:C6	3.07	0.42
1:X:1036:G:C4	1:X:1145:C:H1'	2.54	0.42
1:X:1203:A:OP1	11:I:33:GLY:O	2.38	0.42
1:X:1623:C:C4'	1:X:1624:A:O5'	2.67	0.42
1:X:2291:U:HO2'	6:D:86:GLY:HA3	1.83	0.42
1:X:2852:G:O2'	1:X:2853:U:H5'	2.20	0.42
3:A:119:ASN:HD22	3:A:124:ALA:HB2	1.85	0.42
3:A:251:TRP:O	3:A:256:LYS:NZ	2.41	0.42
3:A:252:GLY:HA3	3:A:256:LYS:CE	2.49	0.42
6:D:118:ASN:HB3	6:D:122:PHE:CZ	2.52	0.42
11:I:99:VAL:HG23	11:I:99:VAL:O	2.19	0.42
14:L:29:LEU:HD23	14:L:89:PHE:CD1	2.55	0.42
15:M:82:PRO:C	15:M:84:ALA:N	2.70	0.42
25:W:47:VAL:HB	25:W:50:LEU:HD12	2.01	0.42
30:4:19:ARG:HD2	30:4:24:LEU:HD13	2.01	0.42
1:X:396:U:C4	1:X:398:C:C6	3.07	0.42
1:X:454:G:C2	1:X:456:C:C2	3.07	0.42
1:X:806:A:OP2	1:X:2055:G:H5'	2.19	0.42
1:X:933:G:H2'	1:X:934:G:C8	2.55	0.42
1:X:1045:G:N2	1:X:1133:G:H1'	2.34	0.42
1:X:1053:G:C6	1:X:1125:G:C2	3.08	0.42
1:X:1174:G:C2	1:X:1175:A:C4	3.07	0.42
1:X:1499:A:C6	1:X:1500:U:N3	2.88	0.42
1:X:1970:G:O2'	1:X:1971:C:H5'	2.20	0.42
1:X:2629:U:OP1	10:H:35:THR:HG21	2.19	0.42
1:X:2790:C:H42	1:X:2806:G:H1	1.66	0.42
1:X:2825:A:N3	1:X:2825:A:C2'	2.80	0.42
5:C:48:ARG:H	5:C:48:ARG:HD2	1.84	0.42
7:E:171:LEU:N	7:E:171:LEU:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:61:ARG:NH2	9:G:61:ARG:HB3	2.35	0.42
9:G:106:TYR:CD2	9:G:106:TYR:O	2.73	0.42
13:K:94:TYR:CD2	13:K:115:LEU:O	2.72	0.42
14:L:47:ARG:C	14:L:49:GLN:H	2.23	0.42
16:N:14:HIS:CD2	16:N:32:TYR:CE2	3.07	0.42
18:P:28:ALA:HB2	18:P:71:VAL:HG22	2.02	0.42
18:P:93:LYS:HB2	18:P:129:ALA:HB3	2.01	0.42
19:Q:5:ASP:O	19:Q:7:LEU:HD12	2.20	0.42
23:U:51:ILE:O	23:U:52:ARG:HD3	2.18	0.42
26:Z:16:ARG:HD2	26:Z:16:ARG:C	2.40	0.42
30:4:19:ARG:HD2	30:4:24:LEU:CD2	2.46	0.42
1:X:98:U:N3	1:X:100:G:N2	2.67	0.42
1:X:128:C:C2'	1:X:129:A:H5"	2.46	0.42
1:X:224:G:N2	1:X:229:G:C6	2.87	0.42
1:X:424:G:H4'	1:X:425:A:OP1	2.19	0.42
1:X:456:C:P	16:N:2:PRO:HD3	2.60	0.42
1:X:659:G:C1'	29:3:46:LYS:HG3	2.49	0.42
1:X:843:G:O4'	1:X:2427:A:C2	2.73	0.42
1:X:1129:A:N6	1:X:1130:U:H3	2.18	0.42
1:X:1631:C:C5	1:X:1633:C:C6	3.07	0.42
1:X:2426:G:H4'	1:X:2427:A:C5'	2.49	0.42
1:X:2508:G:H5"	1:X:2509:A:H5"	2.01	0.42
1:X:2685:A:N1	1:X:2686:C:C2	2.87	0.42
1:X:2768:C:O2	1:X:2784:A:H2	2.02	0.42
3:A:248:VAL:H	3:A:248:VAL:HG13	1.40	0.42
9:G:52:GLY:O	9:G:53:ARG:C	2.55	0.42
9:G:170:PRO:HB2	9:G:171:LEU:H	1.64	0.42
14:L:44:ASP:HB3	14:L:47:ARG:O	2.20	0.42
15:M:56:ALA:HB3	15:M:67:THR:H	1.84	0.42
15:M:82:PRO:O	15:M:83:PHE:C	2.58	0.42
15:M:99:VAL:HG22	15:M:100:ARG:N	2.34	0.42
17:O:11:GLN:HA	17:O:38:LEU:O	2.20	0.42
23:U:53:GLU:HA	23:U:58:LYS:HB2	2.02	0.42
29:3:60:LEU:HA	29:3:63:PRO:HG2	2.00	0.42
1:X:177:U:O4	1:X:225:G:N1	2.53	0.42
1:X:334:G:H2'	5:C:162:ARG:NH1	2.35	0.42
1:X:816:U:C4	1:X:817:A:N7	2.88	0.42
1:X:1099:A:O3'	1:X:1100:G:H8	2.03	0.42
1:X:1357:U:C4'	1:X:1397:A:C6	3.01	0.42
1:X:1386:A:H2'	1:X:1387:G:O4'	2.19	0.42
1:X:1928:G:C6	1:X:1929:U:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2004:U:P	26:Z:12:SER:HG	2.42	0.42
1:X:2036:G:OP1	4:B:144:ARG:HG3	2.20	0.42
1:X:2788:C:O2'	1:X:2789:U:H5'	2.19	0.42
11:I:76:LYS:HG3	11:I:111:SER:HB2	2.02	0.42
14:L:38:ILE:CD1	14:L:39:TYR:N	2.82	0.42
15:M:104:LEU:C	15:M:106:TYR:N	2.73	0.42
16:N:27:SER:HB2	16:N:31:GLN:HG3	2.02	0.42
17:O:38:LEU:HD13	17:O:39:PHE:N	2.35	0.42
18:P:107:ILE:CG2	18:P:117:ILE:HG12	2.50	0.42
21:S:26:LYS:HE3	21:S:26:LYS:HB2	1.80	0.42
22:T:20:TYR:O	22:T:21:LEU:HB2	2.20	0.42
22:T:23:VAL:HA	22:T:38:VAL:HG22	2.02	0.42
1:X:42:G:N2	1:X:450:C:C2	2.88	0.42
1:X:448:C:H5	1:X:449:C:C5	2.37	0.42
1:X:589:C:H4'	16:N:31:GLN:CD	2.40	0.42
1:X:759:C:H1'	1:X:761:G:N2	2.35	0.42
1:X:817:A:C5'	1:X:818:G:OP1	2.68	0.42
1:X:1081:A:H62	1:X:1108:U:H4'	1.84	0.42
1:X:1492:A:N6	1:X:1531:C:C4	2.87	0.42
1:X:1666:G:H1	1:X:1991:C:N4	2.14	0.42
1:X:1703:C:H2'	1:X:1704:G:O4'	2.19	0.42
1:X:1969:G:N2	1:X:1970:G:C4	2.88	0.42
1:X:1988:A:C5'	1:X:1989:C:OP2	2.64	0.42
2:Y:43:G:H5'	2:Y:44:C:H5'	2.01	0.42
2:Y:48:A:N6	2:Y:49:C:C4	2.88	0.42
2:Y:58:G:H5"	2:Y:59:A:OP1	2.19	0.42
3:A:252:GLY:HA3	3:A:256:LYS:HZ1	1.84	0.42
4:B:167:VAL:HG11	4:B:170:LEU:HD21	2.02	0.42
5:C:62:LYS:HD3	5:C:62:LYS:C	2.39	0.42
9:G:106:TYR:CZ	9:G:108:GLY:CA	3.03	0.42
10:H:9:ASP:O	10:H:95:ALA:HB1	2.19	0.42
10:H:104:GLU:OE2	10:H:125:LYS:NZ	2.53	0.42
18:P:27:VAL:HG23	18:P:125:THR:HG22	2.01	0.42
19:Q:30:SER:O	19:Q:33:ALA:HB3	2.19	0.42
20:R:38:LEU:H	20:R:47:VAL:HB	1.84	0.42
1:X:971:A:H61	12:J:83:ARG:NH2	2.13	0.42
1:X:1255:A:C5	1:X:1256:C:C5	3.08	0.42
1:X:1299:A:N6	1:X:1342:U:C2	2.88	0.42
1:X:1379:A:H2'	1:X:1380:C:O4'	2.20	0.42
1:X:1744:G:N2	1:X:1746:A:H3'	2.35	0.42
1:X:1886:G:H2'	1:X:1887:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1947:G:HO2'	1:X:1950:C:P	2.42	0.42
1:X:2329:C:C6	1:X:2329:C:C3'	3.03	0.42
1:X:2722:C:P	30:4:35:ARG:HH11	2.43	0.42
3:A:71:ARG:HH22	3:A:150:PRO:CA	2.30	0.42
3:A:198:GLY:O	3:A:200:ALA:N	2.53	0.42
3:A:245:ARG:HA	3:A:253:LYS:NZ	2.35	0.42
5:C:14:THR:HG22	5:C:15:ILE:N	2.33	0.42
5:C:149:LEU:HD11	5:C:170:LEU:HD22	2.02	0.42
11:I:43:ALA:C	11:I:45:LYS:N	2.72	0.42
16:N:39:LEU:HD23	16:N:39:LEU:HA	1.83	0.42
17:O:72:ARG:HA	17:O:82:ARG:O	2.20	0.42
19:Q:61:LYS:HA	19:Q:71:GLN:O	2.20	0.42
20:R:10:HIS:C	20:R:12:ASP:H	2.22	0.42
1:X:591:G:C3'	1:X:592:G:H8	2.33	0.41
1:X:758:G:H2'	1:X:759:C:OP1	2.20	0.41
1:X:791:G:H5'	3:A:49:ARG:NH2	2.35	0.41
1:X:1455:C:H4'	1:X:1644:G:OP1	2.20	0.41
1:X:1674:C:H2'	1:X:1675:C:H6	1.84	0.41
1:X:2273:C:OP2	14:L:15:ARG:NH2	2.53	0.41
1:X:2312:A:H4'	1:X:2313:G:O5'	2.19	0.41
1:X:2417:U:O2'	1:X:2418:A:H5"	2.20	0.41
10:H:10:VAL:HG23	10:H:17:ARG:C	2.39	0.41
10:H:116:ARG:NH1	15:M:38:LYS:CE	2.83	0.41
14:L:43:ILE:HG22	14:L:44:ASP:N	2.34	0.41
15:M:39:VAL:HG12	15:M:45:THR:CB	2.50	0.41
17:O:12:TYR:HB2	17:O:39:PHE:HB2	2.02	0.41
18:P:89:ARG:HG2	18:P:131:LYS:H	1.84	0.41
26:Z:4:HIS:CD2	26:Z:4:HIS:H	2.38	0.41
1:X:192:G:C4'	1:X:193:A:H4'	2.49	0.41
1:X:428:A:H2'	1:X:429:C:C6	2.55	0.41
1:X:448:C:C5	1:X:449:C:C5	3.07	0.41
1:X:615:C:H41	11:I:100:ARG:NH1	2.18	0.41
1:X:664:C:C6	1:X:666:U:H5	2.38	0.41
1:X:751:G:O2'	1:X:752:G:P	2.78	0.41
1:X:803:C:H4'	1:X:804:C:OP2	2.19	0.41
1:X:861:G:C2	1:X:943:U:H1'	2.55	0.41
1:X:1175:A:C2	1:X:1176:U:N3	2.88	0.41
1:X:1509:A:N7	1:X:1510:A:C5	2.88	0.41
1:X:1750:A:H4'	1:X:2695:C:O4'	2.20	0.41
1:X:1826:U:H4'	1:X:1952:A:C5	2.55	0.41
1:X:1830:C:N3	1:X:1881:U:C5	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1922:U:H5	1:X:1950:C:HO2'	1.66	0.41
1:X:2263:C:OP2	27:1:9:ILE:HD13	2.20	0.41
1:X:2324:G:OP2	27:1:40:TYR:CD2	2.73	0.41
1:X:2737:A:H8	1:X:2737:A:OP1	2.02	0.41
2:Y:7:C:H2'	2:Y:8:C:C6	2.56	0.41
3:A:147:GLU:HG2	3:A:153:GLY:O	2.19	0.41
3:A:198:GLY:O	3:A:199:ASN:C	2.58	0.41
4:B:47:VAL:O	4:B:80:GLU:HA	2.20	0.41
5:C:17:LEU:HA	5:C:18:PRO:HD3	1.81	0.41
14:L:91:ARG:H	14:L:91:ARG:CD	2.33	0.41
15:M:85:SER:HA	15:M:86:PRO:HD3	1.89	0.41
16:N:24:PHE:O	16:N:29:SER:HB3	2.21	0.41
16:N:36:PHE:O	16:N:39:LEU:HB2	2.20	0.41
16:N:82:GLY:HA3	16:N:113:SER:OG	2.20	0.41
18:P:12:LYS:O	18:P:15:LYS:HB2	2.20	0.41
18:P:50:VAL:O	18:P:53:ALA:HB3	2.20	0.41
18:P:81:HIS:HD2	18:P:82:ASN:ND2	2.18	0.41
19:Q:52:GLY:HA3	19:Q:81:ARG:HB3	2.02	0.41
20:R:18:LYS:H	20:R:18:LYS:CD	2.21	0.41
21:S:51:LEU:HD23	21:S:51:LEU:N	2.28	0.41
21:S:120:LEU:C	21:S:120:LEU:CD2	2.88	0.41
28:2:25:LYS:HE2	28:2:25:LYS:CA	2.51	0.41
29:3:13:ARG:NE	29:3:25:PHE:H	2.17	0.41
29:3:53:ALA:O	29:3:54:GLU:C	2.58	0.41
1:X:1769:U:C5	1:X:1775:A:C4	3.08	0.41
1:X:1834:G:C2	1:X:1884:A:C6	3.08	0.41
1:X:2340:C:O3'	29:3:28:GLY:HA2	2.20	0.41
1:X:2617:G:C5	1:X:2755:A:C6	3.07	0.41
1:X:2660:C:C2	1:X:2707:G:N2	2.88	0.41
1:X:2665:G:C2	1:X:2704:U:O2	2.73	0.41
1:X:2695:C:H2'	1:X:2696:A:C8	2.52	0.41
2:Y:91:A:H2'	2:Y:92:G:C8	2.55	0.41
4:B:116:VAL:HG13	4:B:136:ARG:HE	1.85	0.41
5:C:108:ILE:HG23	5:C:112:GLN:HE21	1.85	0.41
6:D:4:LEU:O	6:D:5:LYS:HB3	2.21	0.41
10:H:29:ILE:HG21	10:H:123:PHE:HE1	1.84	0.41
10:H:116:ARG:HH21	15:M:40:ARG:HB2	1.85	0.41
13:K:18:VAL:O	13:K:19:ALA:C	2.56	0.41
14:L:60:LYS:HG3	14:L:64:LYS:HZ3	1.85	0.41
18:P:50:VAL:O	18:P:54:GLU:HG3	2.21	0.41
1:X:99:U:H3'	1:X:100:G:C5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:169:C:H2'	1:X:170:U:H5'	2.03	0.41
1:X:459:A:H2	1:X:466:A:H2'	1.84	0.41
1:X:476:G:O4'	28:2:16:HIS:CE1	2.73	0.41
1:X:578:U:H5"	1:X:579:G:OP2	2.20	0.41
1:X:686:C:H2'	1:X:687:G:H5'	2.02	0.41
1:X:742:G:O2'	1:X:776:G:H4'	2.20	0.41
1:X:771:C:O2'	1:X:772:G:H5'	2.21	0.41
1:X:825:C:C5'	11:I:30:ALA:HB1	2.49	0.41
1:X:968:C:C4	1:X:970:A:C5	3.09	0.41
1:X:1061:A:C2	1:X:2731:G:C2	3.08	0.41
1:X:1277:G:H8	1:X:1277:G:O5'	2.02	0.41
1:X:1354:A:H4'	19:Q:56:MET:HG2	2.02	0.41
1:X:1356:G:H5'	1:X:1614:C:OP2	2.20	0.41
1:X:1744:G:HO2'	1:X:1745:C:H6	1.67	0.41
1:X:1937:G:H1'	1:X:2530:C:H4'	2.02	0.41
1:X:2000:U:O2	26:Z:10:LYS:HB2	2.19	0.41
1:X:2426:G:C8	1:X:2479:U:H6	2.39	0.41
1:X:2651:U:C2'	1:X:2652:G:O5'	2.68	0.41
2:Y:45:C:O2	6:D:90:THR:HB	2.20	0.41
3:A:59:HIS:O	3:A:60:LYS:C	2.58	0.41
3:A:232:HIS:CG	3:A:233:PRO:HD2	2.55	0.41
5:C:150:LEU:HD13	5:C:167:VAL:HB	2.03	0.41
13:K:76:VAL:O	13:K:79:VAL:HG13	2.20	0.41
16:N:74:MET:HE3	16:N:78:THR:HG22	2.02	0.41
21:S:92:VAL:HG22	21:S:93:GLU:N	2.36	0.41
22:T:56:ASP:O	22:T:57:HIS:HB2	2.21	0.41
27:1:17:GLY:O	27:1:18:THR:HB	2.21	0.41
1:X:30:G:C6	1:X:521:U:O2	2.74	0.41
1:X:88:G:C8	1:X:89:A:H8	2.37	0.41
1:X:201:G:H2'	1:X:202:A:C8	2.55	0.41
1:X:404:A:N7	1:X:405:C:C4	2.89	0.41
1:X:788:G:C4	1:X:807:A:C8	3.09	0.41
1:X:1128:G:H3'	1:X:1129:A:C5'	2.51	0.41
1:X:1313:U:H4'	1:X:1314:A:C5'	2.50	0.41
1:X:1380:C:H42	1:X:1799:A:H2	1.68	0.41
1:X:1885:C:C4'	3:A:245:ARG:HD2	2.50	0.41
1:X:2572:U:H2'	1:X:2573:C:C6	2.56	0.41
31:X:2881:LMA:O55	31:X:2881:LMA:C12	2.68	0.41
3:A:122:PRO:HG2	3:A:123:GLU:OE1	2.20	0.41
4:B:124:GLY:HA3	4:B:135:HIS:O	2.20	0.41
5:C:133:PHE:O	5:C:136:TRP:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:158:ARG:O	5:C:159:ARG:C	2.58	0.41
12:J:11:ARG:HB3	12:J:12:LYS:H	1.48	0.41
12:J:59:PHE:O	12:J:60:ARG:C	2.59	0.41
15:M:28:ARG:CB	15:M:29:PRO:CD	2.88	0.41
15:M:33:VAL:CG2	15:M:51:GLU:HB2	2.36	0.41
16:N:25:TRP:O	16:N:28:ARG:HB2	2.21	0.41
17:O:80:TYR:CE2	17:O:82:ARG:CZ	3.03	0.41
18:P:36:ARG:O	18:P:39:ARG:HB2	2.21	0.41
20:R:14:LEU:HD22	20:R:16:PHE:CZ	2.56	0.41
22:T:69:PHE:C	22:T:70:ILE:HG13	2.40	0.41
1:X:459:A:H1'	1:X:461:A:H62	1.85	0.41
1:X:539:A:C6	1:X:2025:A:N3	2.88	0.41
1:X:614:G:C4	1:X:636:G:C2	3.09	0.41
1:X:814:G:OP2	5:C:56:ARG:CZ	2.69	0.41
1:X:931:G:H2'	1:X:932:G:O4'	2.20	0.41
1:X:1049:C:C2	1:X:1129:A:C2	3.08	0.41
1:X:1373:G:H2'	1:X:1374:G:H5'	2.02	0.41
1:X:1467:U:H6	1:X:1467:U:C3'	2.34	0.41
1:X:1607:A:HO2'	1:X:1608:U:H6	1.68	0.41
1:X:1742:G:C6	1:X:1743:C:N4	2.89	0.41
1:X:1770:U:O2	1:X:1774:A:N6	2.54	0.41
1:X:1810:U:OP1	3:A:159:SER:HB3	2.21	0.41
1:X:1830:C:C4	1:X:1881:U:C5	3.09	0.41
1:X:2221:G:H2'	1:X:2222:U:O5'	2.20	0.41
1:X:2382:C:N3	1:X:2394:G:C2	2.88	0.41
1:X:2664:G:C2	1:X:2665:G:C8	3.09	0.41
1:X:2796:A:C2	1:X:2797:G:C5	3.08	0.41
4:B:5:LEU:HD13	4:B:49:ILE:HD13	2.03	0.41
5:C:117:LEU:HD23	5:C:117:LEU:C	2.41	0.41
7:E:7:GLN:H	7:E:8:PRO:CD	2.34	0.41
9:G:49:VAL:HG12	9:G:50:PRO:O	2.20	0.41
12:J:78:LYS:HA	12:J:88:LYS:NZ	2.36	0.41
20:R:22:VAL:HG13	20:R:81:VAL:C	2.38	0.41
20:R:24:VAL:HG11	20:R:28:LYS:O	2.20	0.41
24:V:15:ALA:O	24:V:18:ILE:HB	2.21	0.41
30:4:15:LYS:HB2	30:4:26:ILE:CG1	2.50	0.41
1:X:2:G:O2'	1:X:3:U:H5'	2.20	0.41
1:X:173:A:O2'	1:X:2051:U:H5	2.03	0.41
1:X:646:C:O2'	1:X:650:U:H5"	2.21	0.41
1:X:777:A:N3	3:A:214:ARG:NH1	2.68	0.41
1:X:1268:U:H2'	5:C:66:ASN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1276:U:C1'	26:Z:10:LYS:HG3	2.51	0.41
1:X:1290:A:H5"	13:K:40:LYS:NZ	2.35	0.41
1:X:1312:G:H5"	1:X:1313:U:P	2.61	0.41
1:X:1757:C:O2'	1:X:1758:C:H5'	2.20	0.41
1:X:1926:U:C1'	1:X:1928:G:H5'	2.51	0.41
1:X:1932:G:N2	1:X:1941:C:C2	2.89	0.41
1:X:1970:G:N2	1:X:1971:C:C2	2.89	0.41
1:X:2291:U:H2'	6:D:37:ASN:HD21	1.86	0.41
1:X:2405:A:H4'	1:X:2406:C:OP2	2.21	0.41
1:X:2863:U:O5'	1:X:2863:U:H6	2.04	0.41
3:A:211:GLY:C	3:A:213:SER:N	2.68	0.41
3:A:220:PRO:O	3:A:221:HIS:O	2.38	0.41
3:A:247:PRO:HD3	3:A:253:LYS:HG3	2.03	0.41
4:B:15:TRP:CD1	15:M:86:PRO:HD3	2.56	0.41
4:B:116:VAL:CG2	4:B:136:ARG:CG	2.99	0.41
5:C:74:VAL:HA	5:C:75:PRO:HD3	1.84	0.41
7:E:16:THR:O	7:E:26:VAL:HA	2.21	0.41
7:E:136:ILE:HD12	7:E:136:ILE:N	2.35	0.41
7:E:156:ALA:O	7:E:157:TYR:CG	2.74	0.41
14:L:60:LYS:HZ2	14:L:64:LYS:CE	2.33	0.41
15:M:101:ARG:HG2	15:M:101:ARG:HH21	1.85	0.41
1:X:395:G:N3	1:X:406:G:N2	2.69	0.41
1:X:465:C:C2	1:X:467:U:C5	3.08	0.41
1:X:600:G:H2'	1:X:601:A:OP1	2.21	0.41
1:X:849:G:C5	1:X:850:C:C4	3.09	0.41
1:X:967:G:O6	12:J:17:ARG:CZ	2.69	0.41
1:X:1031:C:O2'	1:X:1032:A:OP2	2.30	0.41
1:X:1265:G:O2'	1:X:1266:G:C8	2.73	0.41
1:X:1773:C:H1'	1:X:2588:U:C5'	2.51	0.41
1:X:1974:U:C2'	1:X:1975:G:H5"	2.51	0.41
1:X:2441:U:H2'	1:X:2442:C:H6	1.83	0.41
1:X:2445:C:N4	1:X:2446:C:N4	2.69	0.41
1:X:2454:C:H42	1:X:2508:G:H22	1.68	0.41
1:X:2668:U:O2	1:X:2693:U:O5'	2.39	0.41
2:Y:58:G:H5"	2:Y:59:A:P	2.60	0.41
3:A:87:PRO:O	3:A:88:ASN:CB	2.65	0.41
3:A:178:LEU:C	3:A:180:SER:H	2.24	0.41
4:B:101:LYS:HA	4:B:170:LEU:O	2.20	0.41
11:I:61:PRO:CD	29:3:27:SER:HB3	2.46	0.41
13:K:37:THR:OG1	13:K:40:LYS:HG3	2.20	0.41
13:K:54:THR:HG22	13:K:55:ALA:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:72:ASP:OD2	13:K:72:ASP:C	2.59	0.41
14:L:10:LYS:O	14:L:14:ARG:HG3	2.20	0.41
14:L:12:ARG:HG3	14:L:13:THR:HG23	2.02	0.41
14:L:73:LYS:O	14:L:74:ALA:C	2.59	0.41
19:Q:68:PHE:O	19:Q:69:ILE:O	2.38	0.41
22:T:43:THR:O	22:T:43:THR:CG2	2.55	0.41
1:X:14:A:C6	1:X:536:A:C2	3.08	0.41
1:X:105:G:H2'	1:X:106:G:H5'	2.02	0.41
1:X:123:A:C2	28:2:10:ARG:HA	2.56	0.41
1:X:334:G:C2	5:C:162:ARG:NH2	2.89	0.41
1:X:496:C:H2'	1:X:497:C:H5'	2.02	0.41
1:X:579:G:H1'	1:X:994:A:N6	2.36	0.41
1:X:638:A:H4'	1:X:639:G:OP1	2.21	0.41
1:X:696:U:H5'	28:2:30:ILE:HD11	2.02	0.41
1:X:872:G:O2'	1:X:928:G:O6	2.36	0.41
1:X:1042:G:H4'	30:4:6:SER:OG	2.21	0.41
1:X:1129:A:C5	1:X:1130:U:N3	2.89	0.41
1:X:1345:G:C5	1:X:1625:A:C6	3.08	0.41
1:X:1399:C:H2'	1:X:1400:A:C8	2.50	0.41
1:X:1433:A:C5	1:X:1595:A:H2	2.39	0.41
1:X:1478:U:C2	1:X:1479:G:C8	3.09	0.41
1:X:1550:C:O2'	1:X:1551:U:H5"	2.20	0.41
1:X:1745:C:C2'	1:X:1746:A:O4'	2.66	0.41
1:X:1770:U:C2	1:X:1774:A:N7	2.89	0.41
1:X:1938:U:O2'	1:X:2531:U:H5'	2.21	0.41
1:X:1976:U:H4'	4:B:128:SER:HB3	2.02	0.41
1:X:1978:U:C2	1:X:1979:C:H5	2.34	0.41
1:X:2015:G:O4'	1:X:2015:G:P	2.79	0.41
1:X:2031:A:C6	1:X:2600:A:N1	2.89	0.41
1:X:2194:A:H3'	1:X:2195:C:C5'	2.41	0.41
1:X:2432:A:H2'	1:X:2433:G:C8	2.55	0.41
1:X:2477:C:O2'	1:X:2478:C:H5'	2.21	0.41
1:X:2505:G:H1'	30:4:1:MET:CB	2.51	0.41
1:X:2594:U:H2'	1:X:2595:C:C6	2.56	0.41
1:X:2673:G:N3	1:X:2674:C:C6	2.89	0.41
1:X:2691:C:O2'	1:X:2692:A:C5'	2.69	0.41
1:X:2736:U:C3'	30:4:19:ARG:HA	2.51	0.41
1:X:2762:G:H2'	1:X:2762:G:N3	2.35	0.41
1:X:2827:G:C6	1:X:2828:C:N3	2.88	0.41
3:A:39:PRO:HA	3:A:62:LEU:HD22	2.03	0.41
3:A:146:LEU:HB3	3:A:156:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:50:GLY:HA2	4:B:77:ILE:O	2.21	0.41
6:D:146:VAL:HB	6:D:147:ASP:H	1.62	0.41
11:I:56:LEU:HB3	29:3:52:LYS:NZ	2.35	0.41
14:L:24:SER:C	14:L:26:ARG:H	2.23	0.41
15:M:5:ILE:N	15:M:5:ILE:HD12	2.36	0.41
15:M:13:LEU:HD12	15:M:13:LEU:N	2.35	0.41
15:M:83:PHE:N	15:M:83:PHE:HD1	2.19	0.41
16:N:14:HIS:CD2	16:N:32:TYR:CD2	3.09	0.41
18:P:37:LYS:O	18:P:40:LEU:N	2.54	0.41
19:Q:62:ARG:HB2	19:Q:63:LYS:H	1.74	0.41
21:S:13:LYS:HB2	21:S:13:LYS:HZ2	1.82	0.41
21:S:149:ALA:HB1	21:S:160:LEU:HD13	2.02	0.41
22:T:12:ASN:HD22	22:T:14:ARG:HD3	1.86	0.41
22:T:18:PRO:O	22:T:19:LYS:O	2.38	0.41
26:Z:30:LEU:HD23	26:Z:30:LEU:HA	1.91	0.41
27:1:14:SER:HB2	27:1:23:THR:N	2.35	0.41
1:X:82:G:H21	1:X:83:A:N6	2.20	0.41
1:X:934:G:H1'	22:T:26:PHE:CD1	2.56	0.41
1:X:965:G:O2'	1:X:2253:A:N1	2.45	0.41
1:X:1147:G:C4	1:X:1148:G:C8	3.09	0.41
1:X:1698:C:H1'	1:X:1753:A:H2'	2.03	0.41
1:X:1923:U:C4'	1:X:1924:C:O5'	2.69	0.41
1:X:2182:A:C2	1:X:2204:A:C2	3.09	0.41
2:Y:83:C:H2'	2:Y:84:G:O4'	2.21	0.41
3:A:219:LYS:HD2	3:A:220:PRO:O	2.20	0.41
4:B:146:THR:CB	4:B:147:PRO:HD2	2.41	0.41
5:C:95:LEU:C	5:C:95:LEU:HD23	2.40	0.41
10:H:20:MET:O	10:H:53:ALA:HB1	2.21	0.41
12:J:17:ARG:O	12:J:18:MET:HB2	2.21	0.41
12:J:68:ARG:O	12:J:102:ARG:NH2	2.54	0.41
14:L:29:LEU:HD12	14:L:41:GLN:O	2.20	0.41
18:P:40:LEU:HD23	18:P:40:LEU:HA	1.87	0.41
20:R:16:PHE:HB3	20:R:82:ALA:HB1	2.02	0.41
24:V:25:LEU:HD13	24:V:46:LEU:CD1	2.48	0.41
27:1:41:ASP:OD2	27:1:46:LYS:HD2	2.21	0.41
29:3:13:ARG:HG3	29:3:13:ARG:O	2.21	0.41
1:X:1033:G:N2	1:X:1035:G:N2	2.69	0.40
1:X:1174:G:N3	1:X:1175:A:C8	2.89	0.40
1:X:1300:A:C8	13:K:106:ASP:OD2	2.74	0.40
1:X:1625:A:H1'	1:X:1632:A:H1'	2.02	0.40
1:X:1672:A:O2'	4:B:115:GLY:HA2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1761:G:H2'	1:X:1762:C:H6	1.86	0.40
1:X:1950:C:C4	1:X:1951:G:N7	2.89	0.40
1:X:2043:A:C1'	1:X:2481:G:O4'	2.69	0.40
1:X:2705:A:N6	1:X:2707:G:N2	2.69	0.40
2:Y:26:G:N3	2:Y:58:G:C6	2.90	0.40
4:B:152:LYS:HB2	9:G:106:TYR:HB3	2.01	0.40
6:D:30:ARG:O	6:D:158:THR:HB	2.20	0.40
10:H:73:VAL:O	10:H:96:ALA:HB1	2.21	0.40
16:N:13:ARG:O	16:N:16:LYS:HB2	2.21	0.40
16:N:72:HIS:CD2	16:N:110:VAL:HG21	2.45	0.40
17:O:5:ILE:HB	17:O:6:GLN:H	1.67	0.40
20:R:5:SER:O	20:R:6:ALA:O	2.39	0.40
20:R:55:THR:OG1	20:R:56:LYS:N	2.53	0.40
1:X:59:G:O6	1:X:62:U:N3	2.55	0.40
1:X:334:G:H4'	1:X:335:A:C5'	2.51	0.40
1:X:573:C:HO2'	1:X:1266:G:H1	1.69	0.40
1:X:760:U:C5	26:Z:3:LYS:CE	3.03	0.40
1:X:769:C:C4	1:X:770:U:C4	3.09	0.40
1:X:824:U:H1'	1:X:1264:C:O4'	2.21	0.40
1:X:1202:U:O2'	1:X:1203:A:H5'	2.21	0.40
1:X:1281:A:H2'	1:X:1282:A:O4'	2.21	0.40
1:X:1475:U:H6	1:X:1475:U:H3'	1.86	0.40
1:X:1978:U:C2'	1:X:1979:C:OP1	2.69	0.40
1:X:2002:A:N7	26:Z:9:LYS:NZ	2.63	0.40
1:X:2041:A:N1	31:X:2881:LMA:C40	2.84	0.40
1:X:2043:A:O2'	1:X:2044:G:H5'	2.20	0.40
1:X:2282:G:N3	1:X:2293:G:N2	2.69	0.40
1:X:2756:A:H3'	1:X:2756:A:OP1	2.21	0.40
3:A:54:PHE:HA	3:A:218:ARG:HH21	1.86	0.40
5:C:23:ASN:HB3	5:C:26:VAL:CG2	2.52	0.40
14:L:99:ARG:HG3	14:L:100:VAL:N	2.36	0.40
15:M:66:PHE:HD2	15:M:83:PHE:HE1	1.65	0.40
18:P:62:ARG:O	18:P:65:SER:HB2	2.20	0.40
20:R:16:PHE:CZ	20:R:46:VAL:CG2	3.04	0.40
27:1:12:MET:HB2	27:1:27:ASN:OD1	2.20	0.40
1:X:75:C:C2'	1:X:76:C:H5'	2.51	0.40
1:X:514:G:N3	1:X:514:G:C2'	2.84	0.40
1:X:617:U:O2	1:X:617:U:O4'	2.40	0.40
1:X:1814:G:H2'	1:X:1815:G:H8	1.86	0.40
1:X:2013:A:H5"	1:X:2014:A:OP1	2.21	0.40
1:X:2273:C:OP1	14:L:95:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2609:G:N3	1:X:2868:G:C2	2.89	0.40
1:X:2665:G:C6	1:X:2666:U:C4	3.09	0.40
1:X:2753:C:H5"	4:B:164:ARG:HG2	2.02	0.40
1:X:2765:C:O2'	1:X:2766:U:H5'	2.21	0.40
4:B:136:ARG:NH2	4:B:157:ALA:HB2	2.37	0.40
11:I:108:LEU:HD22	11:I:120:VAL:HG11	2.03	0.40
12:J:29:ALA:O	12:J:106:GLU:HG3	2.21	0.40
13:K:29:LEU:HD23	13:K:29:LEU:HA	1.90	0.40
15:M:24:LEU:HD11	15:M:34:ARG:NH2	2.37	0.40
20:R:83:LEU:O	20:R:90:LYS:HE2	2.20	0.40
21:S:163:ASP:HA	21:S:164:PRO:HD3	1.88	0.40
24:V:2:LYS:N	24:V:3:PRO:CD	2.84	0.40
1:X:448:C:C5	1:X:449:C:C4	3.03	0.40
1:X:521:U:C4	1:X:522:G:C2	3.10	0.40
1:X:688:A:N6	1:X:689:A:N6	2.69	0.40
1:X:784:U:H2'	1:X:785:U:C6	2.57	0.40
1:X:1468:A:H8	1:X:1468:A:O5'	2.05	0.40
1:X:1537:U:O2'	1:X:1538:A:H5'	2.22	0.40
1:X:1609:G:H2'	1:X:1610:A:O4'	2.21	0.40
1:X:1652:G:H2'	1:X:1653:C:C6	2.56	0.40
1:X:1683:G:C2'	1:X:1684:G:H5'	2.51	0.40
1:X:1725:C:H42	1:X:1741:G:H1	1.70	0.40
1:X:1841:G:H2'	1:X:1842:G:H5'	2.04	0.40
1:X:1947:G:N1	1:X:1950:C:C4	2.89	0.40
1:X:2059:U:H5	1:X:2575:U:O2	2.05	0.40
1:X:2264:C:C4	27:1:28:ARG:NH2	2.89	0.40
1:X:2348:A:O2'	1:X:2349:G:H5'	2.21	0.40
1:X:2614:A:C2	1:X:2764:U:N3	2.90	0.40
1:X:2625:U:H2'	1:X:2626:U:O4'	2.21	0.40
1:X:2817:A:C2	1:X:2851:G:C2	3.10	0.40
1:X:2819:G:H2'	1:X:2820:C:C6	2.55	0.40
2:Y:55:C:H2'	2:Y:56:G:O4'	2.21	0.40
3:A:69:LYS:HG2	3:A:70:ARG:N	2.36	0.40
3:A:132:LEU:HD23	3:A:132:LEU:N	2.36	0.40
3:A:207:LEU:O	3:A:212:ARG:HB3	2.21	0.40
3:A:234:HIS:CE1	3:A:253:LYS:NZ	2.90	0.40
5:C:39:ARG:HH21	5:C:91:TYR:HB2	1.87	0.40
5:C:149:LEU:HD11	5:C:170:LEU:HB2	2.02	0.40
9:G:46:ALA:HB1	9:G:54:LEU:HD22	2.03	0.40
9:G:90:LEU:HD12	9:G:90:LEU:N	2.36	0.40
10:H:4:PRO:O	10:H:5:GLN:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:134:LEU:HD23	10:H:134:LEU:HA	1.81	0.40
12:J:64:LYS:HZ1	12:J:110:VAL:HG13	1.84	0.40
17:O:36:LYS:HE3	17:O:55:THR:C	2.41	0.40
20:R:44:GLN:HE21	20:R:78:ALA:HB2	1.86	0.40
20:R:48:VAL:O	20:R:50:GLY:N	2.54	0.40
22:T:32:LYS:N	22:T:35:ASN:HD22	2.20	0.40
23:U:39:LYS:O	23:U:40:ARG:HB2	2.22	0.40
29:3:13:ARG:HH12	29:3:26:LYS:N	2.19	0.40
1:X:5:A:C2	1:X:2873:G:C2	3.10	0.40
1:X:177:U:H4'	23:U:40:ARG:HG3	2.03	0.40
1:X:1261:G:O2'	16:N:3:ARG:HA	2.22	0.40
1:X:1742:G:C2	1:X:1743:C:N3	2.89	0.40
1:X:1951:G:O2'	1:X:1952:A:O5'	2.30	0.40
1:X:2046:C:C5	1:X:2047:C:C4	3.09	0.40
1:X:2557:G:O2'	1:X:2558:C:H5'	2.21	0.40
1:X:2659:C:C2	1:X:2660:C:C5	3.09	0.40
1:X:2751:C:H2'	1:X:2752:C:H6	1.87	0.40
4:B:49:ILE:HG21	4:B:49:ILE:HD13	1.85	0.40
4:B:116:VAL:CG2	4:B:136:ARG:HG3	2.52	0.40
6:D:41:GLY:HA2	6:D:44:LYS:O	2.21	0.40
9:G:75:ILE:HG23	9:G:140:GLN:HE21	1.86	0.40
10:H:55:VAL:HG12	10:H:56:LYS:N	2.36	0.40
11:I:45:LYS:HE3	11:I:47:ALA:HB3	2.03	0.40
11:I:77:LEU:HD22	11:I:110:ALA:HA	2.03	0.40
12:J:64:LYS:CD	12:J:108:ALA:O	2.70	0.40
18:P:42:VAL:O	18:P:44:VAL:N	2.55	0.40
28:2:34:ARG:HH11	28:2:42:LEU:CG	2.34	0.40
29:3:49:VAL:HB	29:3:52:LYS:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	251/274 (92%)	195 (78%)	44 (18%)	12 (5%)	2 15
4	B	203/211 (96%)	160 (79%)	29 (14%)	14 (7%)	1 7
5	C	192/205 (94%)	143 (74%)	37 (19%)	12 (6%)	1 9
6	D	175/180 (97%)	137 (78%)	32 (18%)	6 (3%)	3 22
7	E	169/185 (91%)	142 (84%)	20 (12%)	7 (4%)	3 18
8	F	61/144 (42%)	48 (79%)	12 (20%)	1 (2%)	9 40
9	G	140/174 (80%)	104 (74%)	27 (19%)	9 (6%)	1 9
10	H	132/134 (98%)	111 (84%)	17 (13%)	4 (3%)	4 25
11	I	132/156 (85%)	82 (62%)	31 (24%)	19 (14%)	0 1
12	J	134/141 (95%)	96 (72%)	27 (20%)	11 (8%)	1 5
13	K	111/116 (96%)	89 (80%)	14 (13%)	8 (7%)	1 6
14	L	102/114 (90%)	73 (72%)	26 (26%)	3 (3%)	4 25
15	M	106/166 (64%)	82 (77%)	18 (17%)	6 (6%)	1 12
16	N	115/118 (98%)	95 (83%)	16 (14%)	4 (4%)	3 21
17	O	92/100 (92%)	68 (74%)	17 (18%)	7 (8%)	1 6
18	P	124/134 (92%)	101 (82%)	18 (14%)	5 (4%)	3 18
19	Q	91/95 (96%)	63 (69%)	19 (21%)	9 (10%)	0 3
20	R	108/115 (94%)	70 (65%)	26 (24%)	12 (11%)	0 2
21	S	173/237 (73%)	135 (78%)	32 (18%)	6 (4%)	3 21
22	T	72/91 (79%)	53 (74%)	18 (25%)	1 (1%)	11 43
23	U	70/81 (86%)	50 (71%)	13 (19%)	7 (10%)	0 3
24	V	63/67 (94%)	55 (87%)	5 (8%)	3 (5%)	2 15
25	W	53/55 (96%)	47 (89%)	6 (11%)	0	100 100
26	Z	55/60 (92%)	42 (76%)	9 (16%)	4 (7%)	1 6
27	1	51/55 (93%)	30 (59%)	15 (29%)	6 (12%)	0 2
28	2	44/47 (94%)	37 (84%)	5 (11%)	2 (4%)	2 16
29	3	57/66 (86%)	34 (60%)	18 (32%)	5 (9%)	1 4
30	4	35/37 (95%)	29 (83%)	6 (17%)	0	100 100
All	All	3111/3558 (87%)	2371 (76%)	557 (18%)	183 (6%)	1 11

All (183) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	220	PRO
3	A	221	HIS
3	A	248	VAL
4	B	135	HIS
4	B	147	PRO
4	B	148	GLY
4	B	202	ALA
5	C	9	GLN
5	C	68	ARG
10	H	42	LYS
10	H	115	ALA
11	I	36	GLY
11	I	58	ALA
12	J	21	ASP
13	K	6	ALA
13	K	91	PRO
13	K	100	VAL
15	M	17	GLU
16	N	5	LYS
16	N	94	VAL
19	Q	59	PRO
19	Q	61	LYS
19	Q	69	ILE
19	Q	83	ALA
20	R	6	ALA
20	R	60	PRO
24	V	3	PRO
27	1	9	ILE
27	1	30	ASN
28	2	42	LEU
29	3	14	ILE
29	3	60	LEU
3	A	47	ARG
3	A	48	GLY
3	A	152	LYS
4	B	123	ALA
4	B	132	LYS
5	C	22	VAL
5	C	121	ASP
7	E	165	VAL
8	F	120	VAL
9	G	68	PRO
9	G	170	PRO

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Mol	Chain	Res	Type
11	I	38	LYS
11	I	44	GLY
11	I	53	ARG
11	I	86	THR
11	I	88	PHE
12	J	13	GLN
12	J	26	ASP
12	J	83	ARG
12	J	136	GLU
13	K	20	LEU
13	K	93	GLY
14	L	45	ASP
15	M	28	ARG
15	M	105	TYR
16	N	8	ILE
17	O	8	GLY
17	O	80	TYR
18	P	32	ARG
18	P	46	ARG
19	Q	63	LYS
19	Q	74	ASP
19	Q	87	SER
20	R	26	SER
20	R	63	THR
20	R	94	VAL
21	S	26	LYS
21	S	91	PRO
22	T	19	LYS
23	U	16	ASN
23	U	31	GLY
23	U	60	VAL
26	Z	37	HIS
27	1	34	LYS
27	1	42	PRO
29	3	31	HIS
3	A	157	ALA
5	C	128	ALA
5	C	159	ARG
7	E	55	PRO
7	E	173	ALA
10	H	27	SER
10	H	116	ARG

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Mol	Chain	Res	Type
11	I	33	GLY
12	J	10	PHE
12	J	17	ARG
13	K	7	GLY
15	M	29	PRO
16	N	92	ARG
17	O	25	LEU
17	O	79	GLN
18	P	43	ASP
20	R	5	SER
21	S	87	THR
21	S	88	TYR
23	U	15	VAL
27	1	31	THR
28	2	8	ASN
29	3	32	GLN
3	A	56	GLY
3	A	126	PRO
3	A	253	LYS
4	B	14	ILE
4	B	122	PHE
4	B	137	ARG
5	C	10	ASN
5	C	67	ALA
6	D	146	VAL
7	E	7	GLN
7	E	12	PRO
9	G	67	ARG
9	G	97	ASP
11	I	30	ALA
11	I	65	PHE
11	I	81	GLN
11	I	91	ASP
12	J	79	PRO
12	J	139	ASP
13	K	13	ASN
14	L	60	LYS
15	M	25	PRO
17	O	24	SER
19	Q	65	VAL
20	R	49	GLU
20	R	85	ASP

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Mol	Chain	Res	Type
21	S	7	PRO
21	S	156	GLU
23	U	30	VAL
23	U	39	LYS
24	V	10	GLN
3	A	55	ILE
3	A	113	THR
4	B	43	GLY
4	B	95	ILE
4	B	115	GLY
4	B	136	ARG
5	C	15	ILE
6	D	21	GLY
6	D	52	LYS
9	G	107	GLN
9	G	108	GLY
9	G	118	ALA
9	G	163	PRO
11	I	37	GLN
11	I	57	ILE
11	I	68	VAL
12	J	111	THR
13	K	56	LYS
14	L	53	ALA
17	O	10	LYS
18	P	20	LEU
20	R	7	GLY
20	R	83	LEU
29	3	13	ARG
6	D	77	PHE
6	D	122	PHE
11	I	63	ARG
12	J	18	MET
15	M	83	PHE
17	O	66	GLY
26	Z	53	ASP
11	I	31	GLY
11	I	61	PRO
18	P	132	GLY
4	B	124	GLY
5	C	78	VAL
6	D	174	GLY

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Mol	Chain	Res	Type
7	E	118	PRO
9	G	64	GLY
23	U	14	VAL
24	V	18	ILE
5	C	175	VAL
20	R	51	VAL
20	R	65	PRO
26	Z	4	HIS
26	Z	5	PRO
5	C	103	GLY
7	E	107	ILE
11	I	122	VAL
19	Q	60	GLY
27	1	49	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	194/215 (90%)	184 (95%)	10 (5%)	23 56
4	B	155/157 (99%)	149 (96%)	6 (4%)	32 65
5	C	154/163 (94%)	147 (96%)	7 (4%)	27 61
6	D	153/156 (98%)	150 (98%)	3 (2%)	55 78
7	E	136/144 (94%)	136 (100%)	0	100 100
8	F	46/107 (43%)	46 (100%)	0	100 100
9	G	118/146 (81%)	115 (98%)	3 (2%)	47 74
10	H	103/103 (100%)	94 (91%)	9 (9%)	10 35
11	I	101/121 (84%)	97 (96%)	4 (4%)	31 64
12	J	110/115 (96%)	108 (98%)	2 (2%)	59 80
13	K	90/93 (97%)	82 (91%)	8 (9%)	9 34
14	L	74/82 (90%)	68 (92%)	6 (8%)	11 39
15	M	94/134 (70%)	87 (93%)	7 (7%)	13 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	N	96/97 (99%)	93 (97%)	3 (3%)	40 70
17	O	75/79 (95%)	72 (96%)	3 (4%)	31 64
18	P	108/115 (94%)	101 (94%)	7 (6%)	17 49
19	Q	75/76 (99%)	70 (93%)	5 (7%)	16 47
20	R	91/96 (95%)	84 (92%)	7 (8%)	13 41
21	S	149/192 (78%)	146 (98%)	3 (2%)	55 78
22	T	55/67 (82%)	53 (96%)	2 (4%)	35 66
23	U	57/66 (86%)	55 (96%)	2 (4%)	36 67
24	V	53/55 (96%)	53 (100%)	0	100 100
25	W	48/48 (100%)	48 (100%)	0	100 100
26	Z	51/53 (96%)	47 (92%)	4 (8%)	12 41
27	1	46/48 (96%)	41 (89%)	5 (11%)	6 25
28	2	39/40 (98%)	33 (85%)	6 (15%)	2 12
29	3	46/52 (88%)	43 (94%)	3 (6%)	17 49
30	4	35/35 (100%)	35 (100%)	0	100 100
All	All	2552/2855 (89%)	2437 (96%)	115 (4%)	27 61

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	44	ARG
3	A	49	ARG
3	A	69	LYS
3	A	165	GLN
3	A	199	ASN
3	A	202	HIS
3	A	209	LYS
3	A	219	LYS
3	A	245	ARG
3	A	246	VAL
4	B	44	TYR
4	B	75	THR
4	B	87	ASP
4	B	119	ARG
4	B	137	ARG
4	B	154	LYS
5	C	31	VAL

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Mol	Chain	Res	Type
5	C	62	LYS
5	C	71	ASP
5	C	74	VAL
5	C	91	TYR
5	C	163	ASN
5	C	180	ILE
6	D	51	ASP
6	D	80	ARG
6	D	112	ARG
9	G	104	THR
9	G	113	GLU
9	G	154	GLU
10	H	1	MET
10	H	8	LEU
10	H	9	ASP
10	H	10	VAL
10	H	23	ARG
10	H	29	ILE
10	H	41	ASN
10	H	81	ILE
10	H	109	ARG
11	I	39	SER
11	I	49	PHE
11	I	53	ARG
11	I	60	LEU
12	J	8	THR
12	J	64	LYS
13	K	3	HIS
13	K	5	LYS
13	K	37	THR
13	K	48	VAL
13	K	71	HIS
13	K	91	PRO
13	K	95	THR
13	K	96	ARG
14	L	31	VAL
14	L	38	ILE
14	L	42	ILE
14	L	45	ASP
14	L	60	LYS
14	L	91	ARG
15	M	5	ILE

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Mol	Chain	Res	Type
15	M	20	HIS
15	M	25	PRO
15	M	31	ASP
15	M	85	SER
15	M	92	THR
15	M	98	LYS
16	N	22	LYS
16	N	30	LYS
16	N	93	LYS
17	O	5	ILE
17	O	18	ASP
17	O	87	ARG
18	P	32	ARG
18	P	36	ARG
18	P	39	ARG
18	P	65	SER
18	P	124	ILE
18	P	125	THR
18	P	126	ILE
19	Q	5	ASP
19	Q	7	LEU
19	Q	12	ILE
19	Q	36	THR
19	Q	62	ARG
20	R	10	HIS
20	R	11	ASN
20	R	15	HIS
20	R	18	LYS
20	R	55	THR
20	R	71	GLN
20	R	112	LYS
21	S	34	LEU
21	S	71	MET
21	S	82	ASP
22	T	15	ASP
22	T	64	ASP
23	U	32	ARG
23	U	78	ILE
26	Z	12	SER
26	Z	23	HIS
26	Z	41	LEU
26	Z	58	LEU

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Mol	Chain	Res	Type
27	1	8	ILE
27	1	15	SER
27	1	34	LYS
27	1	51	ARG
27	1	54	LYS
28	2	5	TYR
28	2	10	ARG
28	2	12	ARG
28	2	14	LYS
28	2	15	THR
28	2	44	VAL
29	3	31	HIS
29	3	39	ASP
29	3	46	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	155	GLN
3	A	167	GLN
3	A	199	ASN
5	C	132	ASN
5	C	163	ASN
5	C	176	ASN
6	D	37	ASN
7	E	61	HIS
9	G	73	ASN
9	G	107	GLN
9	G	129	HIS
9	G	145	HIS
10	H	46	HIS
12	J	46	ASN
12	J	47	GLN
13	K	24	GLN
14	L	41	GLN
14	L	97	HIS
16	N	14	HIS
16	N	37	GLN
16	N	72	HIS
16	N	81	ASN
17	O	88	GLN
18	P	73	ASN

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Mol	Chain	Res	Type
18	P	81	HIS
18	P	82	ASN
20	R	29	HIS
20	R	71	GLN
21	S	121	GLN
22	T	12	ASN
22	T	35	ASN
26	Z	29	ASN
26	Z	44	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2647/2880 (91%)	473 (17%)	54 (2%)
2	Y	119/123 (96%)	18 (15%)	0
All	All	2766/3003 (92%)	491 (17%)	54 (1%)

All (491) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	13	A
1	X	14	A
1	X	34	U
1	X	35	G
1	X	39	C
1	X	45	C
1	X	49	U
1	X	59	G
1	X	63	A
1	X	70	A
1	X	74	G
1	X	76	C
1	X	83	A
1	X	87	G
1	X	88	G
1	X	89	A
1	X	90	G
1	X	98	U
1	X	100	G
1	X	101	A

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Mol	Chain	Res	Type
1	X	111	G
1	X	116	A
1	X	118	U
1	X	123	A
1	X	129	A
1	X	136	A
1	X	143	A
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	178	C
1	X	193	A
1	X	199	A
1	X	206	U
1	X	210	A
1	X	219	G
1	X	225	G
1	X	226	C
1	X	229	G
1	X	242	A
1	X	243	G
1	X	304	A
1	X	305	A
1	X	312	G
1	X	318	G
1	X	323	G
1	X	333	A
1	X	334	G
1	X	335	A
1	X	340	G
1	X	342	G
1	X	343	A
1	X	399	G
1	X	400	U
1	X	414	A
1	X	418	C
1	X	424	G
1	X	425	A
1	X	441	A

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Mol	Chain	Res	Type
1	X	456	C
1	X	460	U
1	X	463	C
1	X	467	U
1	X	468	A
1	X	469	G
1	X	482	A
1	X	484	G
1	X	491	A
1	X	492	G
1	X	497	C
1	X	515	A
1	X	537	C
1	X	538	A
1	X	539	A
1	X	540	G
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	555	U
1	X	556	A
1	X	557	U
1	X	572	G
1	X	578	U
1	X	581	A
1	X	582	G
1	X	583	C
1	X	584	A
1	X	587	A
1	X	595	A
1	X	602	C
1	X	613	A
1	X	614	G
1	X	624	A
1	X	625	A
1	X	626	A
1	X	627	A
1	X	628	A
1	X	631	G
1	X	633	G
1	X	636	G

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Mol	Chain	Res	Type
1	X	648	A
1	X	649	G
1	X	652	C
1	X	654	A
1	X	655	A
1	X	657	A
1	X	662	G
1	X	665	A
1	X	666	U
1	X	669	G
1	X	682	G
1	X	683	A
1	X	699	G
1	X	741	G
1	X	743	A
1	X	748	A
1	X	751	G
1	X	752	G
1	X	753	U
1	X	759	C
1	X	760	U
1	X	761	G
1	X	765	C
1	X	766	A
1	X	777	A
1	X	781	G
1	X	789	G
1	X	790	A
1	X	795	A
1	X	797	A
1	X	798	G
1	X	803	C
1	X	804	C
1	X	805	G
1	X	806	A
1	X	807	A
1	X	818	G
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	859	U

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Mol	Chain	Res	Type
1	X	919	U
1	X	921	A
1	X	922	A
1	X	926	C
1	X	939	C
1	X	940	G
1	X	944	A
1	X	952	A
1	X	956	A
1	X	957	G
1	X	969	U
1	X	970	A
1	X	972	C
1	X	983	G
1	X	984	A
1	X	985	G
1	X	994	A
1	X	1006	C
1	X	1007	A
1	X	1016	C
1	X	1019	U
1	X	1023	U
1	X	1032	A
1	X	1033	G
1	X	1037	U
1	X	1044	U
1	X	1051	U
1	X	1054	C
1	X	1056	U
1	X	1057	A
1	X	1058	G
1	X	1060	C
1	X	1070	G
1	X	1078	A
1	X	1081	A
1	X	1082	G
1	X	1087	C
1	X	1090	C
1	X	1097	A
1	X	1098	G
1	X	1099	A
1	X	1108	U

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Mol	Chain	Res	Type
1	X	1119	U
1	X	1123	G
1	X	1128	G
1	X	1129	A
1	X	1142	G
1	X	1145	C
1	X	1146	G
1	X	1148	G
1	X	1149	G
1	X	1152	C
1	X	1153	A
1	X	1167	A
1	X	1168	G
1	X	1183	C
1	X	1192	A
1	X	1220	G
1	X	1223	G
1	X	1224	A
1	X	1249	G
1	X	1250	A
1	X	1266	G
1	X	1269	G
1	X	1275	A
1	X	1278	A
1	X	1279	G
1	X	1282	A
1	X	1284	G
1	X	1285	A
1	X	1288	A
1	X	1289	A
1	X	1299	A
1	X	1301	U
1	X	1313	U
1	X	1314	A
1	X	1325	U
1	X	1326	U
1	X	1340	C
1	X	1342	U
1	X	1345	G
1	X	1358	C
1	X	1359	G
1	X	1378	A

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Mol	Chain	Res	Type
1	X	1381	G
1	X	1391	A
1	X	1392	U
1	X	1393	G
1	X	1398	G
1	X	1405	A
1	X	1409	U
1	X	1413	U
1	X	1428	G
1	X	1430	G
1	X	1432	G
1	X	1434	U
1	X	1440	G
1	X	1442	C
1	X	1443	G
1	X	1460	G
1	X	1465	G
1	X	1468	A
1	X	1469	U
1	X	1470	G
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	1506	C
1	X	1528	C
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	1570	C
1	X	1571	G
1	X	1574	A
1	X	1575	C
1	X	1585	A
1	X	1601	U
1	X	1602	G
1	X	1608	U

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Mol	Chain	Res	Type
1	X	1619	A
1	X	1624	A
1	X	1625	A
1	X	1626	A
1	X	1632	A
1	X	1634	A
1	X	1635	G
1	X	1648	C
1	X	1651	U
1	X	1656	U
1	X	1657	A
1	X	1665	C
1	X	1668	G
1	X	1677	C
1	X	1686	A
1	X	1691	G
1	X	1692	C
1	X	1701	C
1	X	1710	U
1	X	1712	G
1	X	1714	A
1	X	1717	A
1	X	1718	A
1	X	1747	G
1	X	1754	G
1	X	1755	G
1	X	1764	A
1	X	1775	A
1	X	1782	A
1	X	1790	G
1	X	1791	C
1	X	1793	A
1	X	1801	C
1	X	1802	A
1	X	1807	A
1	X	1808	C
1	X	1812	U
1	X	1821	A
1	X	1825	C
1	X	1831	G
1	X	1842	G
1	X	1868	A

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Mol	Chain	Res	Type
1	X	1884	A
1	X	1910	A
1	X	1919	A
1	X	1920	A
1	X	1921	A
1	X	1922	U
1	X	1923	U
1	X	1924	C
1	X	1927	U
1	X	1928	G
1	X	1938	U
1	X	1939	U
1	X	1947	G
1	X	1949	A
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1965	U
1	X	1975	G
1	X	1976	U
1	X	1979	C
1	X	1980	A
1	X	1988	A
1	X	2006	G
1	X	2009	U
1	X	2014	A
1	X	2015	G
1	X	2016	A
1	X	2017	U
1	X	2019	C
1	X	2026	C
1	X	2029	G
1	X	2038	C
1	X	2039	G
1	X	2043	A
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2075	U
1	X	2083	G

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Mol	Chain	Res	Type
1	X	2171	U
1	X	2181	A
1	X	2190	A
1	X	2191	A
1	X	2192	U
1	X	2195	C
1	X	2199	C
1	X	2200	G
1	X	2205	C
1	X	2218	G
1	X	2238	G
1	X	2241	U
1	X	2242	C
1	X	2246	A
1	X	2247	A
1	X	2259	G
1	X	2262	C
1	X	2265	A
1	X	2266	A
1	X	2272	A
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A
1	X	2298	U
1	X	2300	G
1	X	2301	A
1	X	2306	A
1	X	2313	G
1	X	2315	A
1	X	2324	G
1	X	2325	A
1	X	2326	C
1	X	2362	G
1	X	2364	C
1	X	2386	G
1	X	2396	C
1	X	2398	U
1	X	2402	U
1	X	2404	A
1	X	2405	A

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Mol	Chain	Res	Type
1	X	2407	G
1	X	2410	U
1	X	2418	A
1	X	2420	C
1	X	2426	G
1	X	2427	A
1	X	2452	U
1	X	2455	A
1	X	2458	U
1	X	2470	U
1	X	2471	U
1	X	2477	C
1	X	2481	G
1	X	2482	A
1	X	2483	U
1	X	2484	G
1	X	2485	U
1	X	2497	A
1	X	2498	U
1	X	2501	U
1	X	2528	G
1	X	2545	A
1	X	2546	G
1	X	2548	G
1	X	2553	G
1	X	2561	G
1	X	2564	U
1	X	2565	C
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2591	C
1	X	2594	U
1	X	2608	A
1	X	2609	G
1	X	2613	A
1	X	2634	G
1	X	2650	G
1	X	2664	G
1	X	2668	U
1	X	2691	C
1	X	2692	A

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Mol	Chain	Res	Type
1	X	2693	U
1	X	2694	G
1	X	2706	U
1	X	2713	A
1	X	2730	A
1	X	2731	G
1	X	2732	C
1	X	2737	A
1	X	2744	A
1	X	2745	A
1	X	2757	G
1	X	2758	A
1	X	2759	U
1	X	2760	G
1	X	2761	A
1	X	2770	A
1	X	2771	C
1	X	2782	G
1	X	2783	U
1	X	2792	C
1	X	2795	A
1	X	2796	A
1	X	2807	U
1	X	2808	U
1	X	2809	A
1	X	2814	G
1	X	2825	A
1	X	2842	C
1	X	2847	G
1	X	2850	U
1	X	2867	G
1	X	2868	G
2	Y	4	C
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	43	G
2	Y	44	C

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Mol	Chain	Res	Type
2	Y	46	G
2	Y	47	A
2	Y	59	A
2	Y	69	G
2	Y	102	A
2	Y	110	U
2	Y	111	C
2	Y	112	A

All (54) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	33	C
1	X	38	G
1	X	48	A
1	X	62	U
1	X	334	G
1	X	342	G
1	X	467	U
1	X	538	A
1	X	751	G
1	X	759	C
1	X	760	U
1	X	780	U
1	X	788	G
1	X	789	G
1	X	969	U
1	X	983	G
1	X	984	A
1	X	1031	C
1	X	1053	G
1	X	1096	A
1	X	1141	U
1	X	1182	U
1	X	1223	G
1	X	1312	G
1	X	1313	U
1	X	1357	U
1	X	1391	A
1	X	1441	A
1	X	1442	C
1	X	1496	G

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Mol	Chain	Res	Type
1	X	1601	U
1	X	1607	A
1	X	1623	C
1	X	1685	A
1	X	1781	C
1	X	1790	G
1	X	1811	A
1	X	1923	U
1	X	1938	U
1	X	1975	G
1	X	2015	G
1	X	2018	G
1	X	2044	G
1	X	2045	A
1	X	2204	A
1	X	2312	A
1	X	2404	A
1	X	2409	A
1	X	2426	G
1	X	2692	A
1	X	2705	A
1	X	2736	U
1	X	2756	A
1	X	2824	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 212 ligands modelled in this entry, 211 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	$\#\|Z\| > 2$
31	LMA	X	2881	-	58,60,60	4.94	26 (44%)	75,90,90	1.30	5 (6%)

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
31	LMA	X	2881	-	-	20/80/115/115	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	2881	LMA	C30-C2	-19.79	1.10	1.53
31	X	2881	LMA	C2-C1	-17.00	1.13	1.51
31	X	2881	LMA	O53-C8	-10.30	1.25	1.43
31	X	2881	LMA	O2-C13	8.52	1.57	1.44
31	X	2881	LMA	C35-C12	-8.22	1.36	1.53
31	X	2881	LMA	C33-C8	-7.31	1.41	1.52
31	X	2881	LMA	C7-C6	-7.19	1.44	1.54
31	X	2881	LMA	C19-C16	-6.15	1.38	1.52
31	X	2881	LMA	C32-C6	-6.04	1.38	1.53
31	X	2881	LMA	C8-C9	-5.87	1.41	1.54
31	X	2881	LMA	O5-C16	-5.24	1.34	1.44
31	X	2881	LMA	C16-C17	-5.20	1.41	1.53
31	X	2881	LMA	C40-C23	-4.85	1.43	1.53
31	X	2881	LMA	O55-C54	4.79	1.38	1.20
31	X	2881	LMA	C6-C5	4.54	1.61	1.53
31	X	2881	LMA	O52-C51	4.44	1.37	1.20
31	X	2881	LMA	O51-C17	-4.17	1.37	1.45
31	X	2881	LMA	O2-C1	3.76	1.43	1.34
31	X	2881	LMA	C2-C3	3.71	1.63	1.55
31	X	2881	LMA	C12-C13	-3.68	1.44	1.54
31	X	2881	LMA	O17-C24	3.15	1.51	1.43
31	X	2881	LMA	O3-C3	2.72	1.50	1.43
31	X	2881	LMA	O4-C18	2.24	1.49	1.44
31	X	2881	LMA	C4-C5	2.18	1.59	1.54
31	X	2881	LMA	C15-C16	2.08	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	2881	LMA	O12-C54	2.02	1.39	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	X	2881	LMA	O12-C54-C56	4.58	119.52	111.09
31	X	2881	LMA	O51-C51-C53	4.56	119.48	111.09
31	X	2881	LMA	O7-C5-C4	3.88	112.90	108.22
31	X	2881	LMA	C3-C2-C1	-2.76	104.38	110.01
31	X	2881	LMA	C25-C24-C23	-2.45	106.55	113.08

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	X	2881	LMA	C3-C4-C5-C6
31	X	2881	LMA	C3-C4-C5-O7
31	X	2881	LMA	C31-C4-C5-C6
31	X	2881	LMA	C12-C11-O12-C54
31	X	2881	LMA	C13-C36-C57-O57
31	X	2881	LMA	C13-C36-C57-C58
31	X	2881	LMA	C37-C36-C57-O57
31	X	2881	LMA	C37-C36-C57-C58
31	X	2881	LMA	C53-C51-O51-C17
31	X	2881	LMA	O52-C51-O51-C17
31	X	2881	LMA	C31-C4-C5-O7
31	X	2881	LMA	C25-C24-O17-C29
31	X	2881	LMA	C10-C11-O12-C54
31	X	2881	LMA	C6-C7-C8-C9
31	X	2881	LMA	C12-C13-C36-C57
31	X	2881	LMA	O9-C22-O7-C5
31	X	2881	LMA	C6-C7-C8-C33
31	X	2881	LMA	C15-C16-O5-C20
31	X	2881	LMA	C19-C16-O5-C20
31	X	2881	LMA	C6-C7-C8-O53

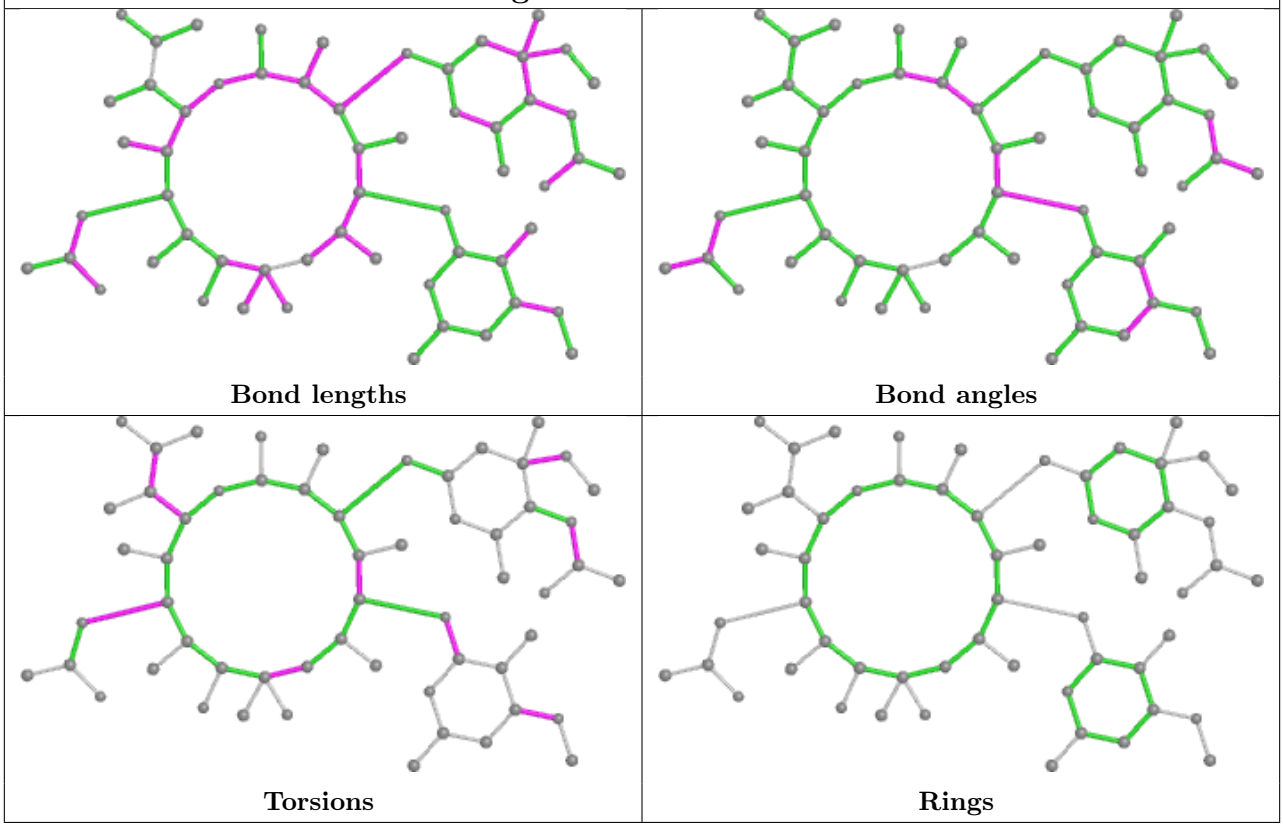
There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	X	2881	LMA	13	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 LMA X 2881



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	2657/2880 (92%)	-0.13	75 (2%) 53 41	32, 91, 207, 392	0
2	Y	120/123 (97%)	0.08	2 (1%) 70 60	85, 155, 211, 300	0
3	A	253/274 (92%)	0.42	15 (5%) 22 15	54, 119, 183, 297	0
4	B	205/211 (97%)	-0.34	3 (1%) 73 64	22, 64, 130, 298	0
5	C	194/205 (94%)	0.19	14 (7%) 15 10	44, 117, 220, 268	0
6	D	177/180 (98%)	0.88	25 (14%) 2 2	146, 209, 280, 370	0
7	E	171/185 (92%)	0.24	11 (6%) 19 13	86, 149, 209, 245	0
8	F	63/144 (43%)	3.09	43 (68%) 0 0	180, 261, 394, 440	0
9	G	142/174 (81%)	0.27	8 (5%) 24 15	55, 101, 188, 266	0
10	H	134/134 (100%)	-0.48	1 (0%) 87 83	35, 61, 108, 204	0
11	I	134/156 (85%)	0.65	15 (11%) 5 4	64, 145, 237, 367	0
12	J	136/141 (96%)	0.17	7 (5%) 28 18	76, 108, 190, 272	0
13	K	113/116 (97%)	-0.65	0 100 100	27, 46, 79, 105	0
14	L	104/114 (91%)	0.54	11 (10%) 6 5	117, 160, 248, 306	0
15	M	108/166 (65%)	-0.33	3 (2%) 53 41	36, 60, 135, 241	0
16	N	117/118 (99%)	-0.12	4 (3%) 45 33	44, 88, 156, 279	0
17	O	94/100 (94%)	0.15	6 (6%) 19 13	58, 119, 195, 238	0
18	P	126/134 (94%)	-0.40	0 100 100	29, 59, 118, 200	0
19	Q	93/95 (97%)	0.04	2 (2%) 62 52	59, 107, 182, 273	0
20	R	110/115 (95%)	0.66	21 (19%) 1 1	68, 127, 234, 359	0
21	S	175/237 (73%)	0.93	34 (19%) 1 1	112, 169, 237, 314	0
22	T	74/91 (81%)	0.63	13 (17%) 1 1	82, 123, 199, 271	0
23	U	72/81 (88%)	1.79	20 (27%) 0 0	89, 155, 302, 332	0
24	V	65/67 (97%)	0.29	4 (6%) 20 13	94, 126, 205, 256	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	55/55 (100%)	0.08	2 (3%) 42 31	73, 102, 166, 177	0
26	Z	57/60 (95%)	-0.15	2 (3%) 44 32	31, 63, 108, 191	0
27	1	53/55 (96%)	1.55	17 (32%) 0 0	106, 171, 261, 319	0
28	2	46/47 (97%)	0.22	3 (6%) 18 12	56, 85, 154, 195	0
29	3	59/66 (89%)	1.58	21 (35%) 0 0	97, 150, 276, 316	0
30	4	37/37 (100%)	6.38	35 (94%) 0 0	133, 223, 289, 323	0
All	All	5944/6561 (90%)	0.16	417 (7%) 16 11	22, 105, 230, 440	0

All (417) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	28	GLY	25.4
30	4	25	VAL	14.2
8	F	113	PRO	14.0
30	4	17	VAL	13.9
30	4	24	LEU	12.9
30	4	13	ASN	12.7
3	A	204	ASN	12.4
8	F	114	ASP	11.2
21	S	91	PRO	10.0
30	4	6	SER	9.4
30	4	23	VAL	9.3
23	U	27	ASP	9.2
27	1	35	LEU	9.1
30	4	35	ARG	8.9
8	F	125	ASN	8.5
6	D	75	SER	8.4
21	S	15	ASP	8.4
1	X	1095	A	8.2
30	4	4	ARG	8.2
6	D	43	SER	8.1
23	U	26	ALA	7.9
23	U	29	GLY	7.8
30	4	34	GLN	7.8
8	F	112	MET	7.6
5	C	19	LEU	7.2
30	4	5	SER	7.0
30	4	27	CYS	7.0
23	U	47	HIS	7.0
30	4	12	ASP	7.0

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Mol	Chain	Res	Type	RSRZ
19	Q	64	ARG	7.0
8	F	97	GLY	6.8
30	4	26	ILE	6.7
30	4	21	GLY	6.5
30	4	16	VAL	6.5
1	X	1080	A	6.4
30	4	3	VAL	6.4
30	4	28	SER	6.3
1	X	1085	G	6.2
30	4	29	ASN	6.0
22	T	73	GLY	6.0
29	3	50	LEU	6.0
1	X	665	A	5.9
30	4	36	GLN	5.8
3	A	251	TRP	5.8
30	4	11	CYS	5.8
1	X	1115	C	5.7
4	B	205	SER	5.7
8	F	123	ALA	5.7
1	X	1106	A	5.7
6	D	145	MET	5.6
30	4	1	MET	5.6
30	4	37	GLY	5.6
6	D	45	GLU	5.6
1	X	1107	A	5.5
6	D	76	ASN	5.4
27	1	45	LYS	5.4
6	D	147	ASP	5.3
21	S	23	ALA	5.2
30	4	7	VAL	5.2
5	C	165	SER	5.1
9	G	156	HIS	5.1
27	1	32	GLN	5.1
30	4	20	HIS	5.1
11	I	56	LEU	5.0
30	4	33	LYS	5.0
1	X	248	A	5.0
6	D	142	THR	5.0
30	4	14	CYS	5.0
21	S	92	VAL	5.0
20	R	57	ASN	5.0
30	4	10	MET	5.0

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Mol	Chain	Res	Type	RSRZ
30	4	22	ARG	4.9
30	4	15	LYS	4.8
20	R	102	LYS	4.8
8	F	120	VAL	4.8
22	T	85	GLN	4.8
12	J	84	MET	4.8
6	D	71	LYS	4.8
21	S	31	SER	4.7
6	D	74	ILE	4.7
1	X	1086	C	4.7
29	3	9	MET	4.7
11	I	54	SER	4.7
1	X	2287	G	4.7
27	1	23	THR	4.7
3	A	250	PRO	4.7
6	D	143	TYR	4.6
24	V	66	GLN	4.6
3	A	243	ALA	4.6
16	N	88	ILE	4.6
3	A	161	GLY	4.6
23	U	12	ASN	4.5
8	F	101	TRP	4.5
8	F	136	VAL	4.5
21	S	12	GLN	4.4
17	O	64	GLY	4.4
20	R	67	GLY	4.4
1	X	1114	A	4.4
1	X	1104	G	4.4
22	T	18	PRO	4.4
30	4	32	HIS	4.4
27	1	47	HIS	4.3
21	S	128	ARG	4.3
29	3	55	TRP	4.3
8	F	85	GLY	4.2
27	1	27	ASN	4.2
1	X	1072	U	4.2
22	T	15	ASP	4.2
22	T	16	SER	4.2
11	I	36	GLY	4.1
27	1	52	GLU	4.1
21	S	76	ARG	4.1
1	X	558	G	4.1

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Mol	Chain	Res	Type	RSRZ
9	G	97	ASP	4.0
21	S	94	VAL	4.0
21	S	30	VAL	4.0
23	U	52	ARG	4.0
23	U	30	VAL	4.0
23	U	13	LEU	4.0
8	F	76	TYR	3.9
6	D	120	ASN	3.9
14	L	35	SER	3.9
20	R	58	VAL	3.8
1	X	1089	C	3.8
8	F	90	THR	3.8
22	T	13	GLY	3.8
7	E	25	LYS	3.7
1	X	1079	G	3.7
27	1	13	GLU	3.7
8	F	94	ALA	3.7
1	X	2190	A	3.7
16	N	91	ASN	3.7
1	X	1068	A	3.6
1	X	1077	U	3.6
21	S	22	VAL	3.6
1	X	1057	A	3.6
20	R	112	LYS	3.6
21	S	55	THR	3.6
11	I	74	VAL	3.6
29	3	33	ASN	3.6
23	U	46	LEU	3.5
30	4	2	LYS	3.5
8	F	99	LEU	3.5
24	V	4	SER	3.5
12	J	27	TYR	3.5
5	C	44	SER	3.5
27	1	14	SER	3.5
3	A	220	PRO	3.5
29	3	44	LYS	3.5
1	X	358	C	3.5
8	F	111	LYS	3.4
27	1	36	GLU	3.4
6	D	81	GLN	3.4
21	S	113	VAL	3.4
3	A	85	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
8	F	119	SER	3.4
22	T	71	ASN	3.4
8	F	132	ARG	3.4
6	D	42	SER	3.4
8	F	121	GLU	3.3
6	D	125	ARG	3.3
29	3	21	LYS	3.3
5	C	48	ARG	3.3
6	D	144	ASP	3.3
23	U	16	ASN	3.3
5	C	167	VAL	3.3
3	A	268	ASP	3.3
20	R	66	GLN	3.3
6	D	18	GLN	3.2
1	X	1081	A	3.2
11	I	52	GLY	3.2
21	S	14	LEU	3.2
21	S	21	ALA	3.2
29	3	61	MET	3.2
8	F	91	PRO	3.2
20	R	52	ASN	3.2
20	R	94	VAL	3.2
27	1	31	THR	3.2
10	H	27	SER	3.2
1	X	1108	U	3.2
8	F	129	GLY	3.2
7	E	51	LEU	3.1
8	F	92	ASN	3.1
5	C	193	LEU	3.1
9	G	159	SER	3.1
22	T	17	ASN	3.1
11	I	57	ILE	3.1
29	3	43	GLY	3.1
20	R	100	ASP	3.1
8	F	133	SER	3.1
1	X	1552	C	3.1
1	X	1105	U	3.1
14	L	63	ASN	3.1
27	1	24	THR	3.0
21	S	83	PHE	3.0
8	F	78	ILE	3.0
3	A	32	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
5	C	47	THR	3.0
3	A	203	LYS	3.0
1	X	1734	C	3.0
1	X	1120	C	3.0
1	X	2290	A	3.0
17	O	36	LYS	3.0
1	X	1037	U	3.0
30	4	18	ARG	3.0
12	J	136	GLU	3.0
3	A	221	HIS	3.0
1	X	1067	G	3.0
1	X	1913	G	3.0
1	X	1191	G	2.9
14	L	62	GLY	2.9
22	T	14	ARG	2.9
21	S	173	PRO	2.9
1	X	732	G	2.9
29	3	10	ALA	2.9
6	D	20	PHE	2.9
7	E	23	VAL	2.9
17	O	46	VAL	2.9
21	S	77	ALA	2.9
7	E	62	ARG	2.9
1	X	1184	G	2.9
29	3	39	ASP	2.9
14	L	64	LYS	2.9
11	I	31	GLY	2.9
29	3	48	PHE	2.9
6	D	72	LYS	2.9
29	3	54	GLU	2.9
21	S	11	LYS	2.9
1	X	601	A	2.9
5	C	192	ALA	2.9
6	D	46	ASP	2.8
17	O	39	PHE	2.8
4	B	135	HIS	2.8
8	F	96	VAL	2.8
1	X	2015	G	2.8
24	V	5	GLU	2.8
25	W	33	GLU	2.8
8	F	81	ALA	2.8
21	S	24	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
22	T	20	TYR	2.8
29	3	14	ILE	2.8
21	S	147	ILE	2.8
2	Y	68	A	2.8
8	F	95	LYS	2.8
29	3	51	ALA	2.8
23	U	61	TRP	2.8
8	F	77	LEU	2.8
29	3	38	GLY	2.8
14	L	55	SER	2.7
20	R	61	SER	2.7
21	S	165	GLU	2.7
8	F	80	LYS	2.7
8	F	84	ILE	2.7
27	1	2	ALA	2.7
8	F	127	VAL	2.7
30	4	9	LYS	2.7
20	R	60	PRO	2.7
1	X	1602	G	2.7
3	A	153	GLY	2.7
8	F	108	ALA	2.7
6	D	40	LEU	2.6
1	X	304	A	2.6
1	X	1119	U	2.6
21	S	32	PHE	2.6
8	F	104	VAL	2.6
12	J	28	VAL	2.6
21	S	86	VAL	2.6
1	X	1912	G	2.6
1	X	1076	U	2.6
23	U	8	THR	2.6
8	F	122	ALA	2.6
1	X	2289	A	2.6
8	F	110	THR	2.6
2	Y	4	C	2.6
20	R	71	GLN	2.6
7	E	37	TYR	2.6
5	C	45	THR	2.6
30	4	30	VAL	2.6
8	F	105	LEU	2.6
1	X	247	A	2.6
1	X	1522	C	2.6

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Mol	Chain	Res	Type	RSRZ
21	S	174	PRO	2.6
9	G	39	GLN	2.5
27	1	22	TYR	2.5
1	X	302	U	2.5
9	G	129	HIS	2.5
6	D	146	VAL	2.5
23	U	54	ASN	2.5
14	L	65	THR	2.5
14	L	111	GLY	2.5
1	X	667	U	2.5
11	I	55	ARG	2.5
11	I	97	ARG	2.5
23	U	25	ARG	2.5
27	1	51	ARG	2.5
12	J	112	GLU	2.5
1	X	1078	A	2.5
1	X	1109	A	2.5
11	I	33	GLY	2.5
29	3	13	ARG	2.5
15	M	29	PRO	2.5
21	S	85	MET	2.5
1	X	1055	A	2.5
21	S	145	ASP	2.5
20	R	69	GLN	2.5
22	T	66	LYS	2.5
8	F	124	ALA	2.5
5	C	59	TYR	2.5
29	3	7	HIS	2.5
1	X	1098	G	2.4
29	3	45	GLY	2.4
22	T	84	ALA	2.4
1	X	2085	G	2.4
21	S	125	PRO	2.4
8	F	86	LYS	2.4
8	F	102	ASP	2.4
17	O	47	PHE	2.4
14	L	56	SER	2.4
20	R	81	VAL	2.4
1	X	1909	U	2.4
1	X	1090	C	2.4
7	E	119	ALA	2.4
1	X	1733	U	2.4

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Mol	Chain	Res	Type	RSRZ
21	S	124	ALA	2.4
1	X	1084	A	2.3
9	G	109	GLY	2.3
1	X	2087	U	2.3
7	E	5	GLY	2.3
26	Z	37	HIS	2.3
4	B	94	ASP	2.3
17	O	23	GLU	2.3
7	E	61	HIS	2.3
1	X	2082	C	2.3
8	F	107	ILE	2.3
29	3	63	PRO	2.3
5	C	166	TRP	2.3
20	R	77	HIS	2.3
15	M	40	ARG	2.3
1	X	2174	G	2.3
27	1	19	GLY	2.3
21	S	93	GLU	2.3
11	I	46	GLY	2.3
23	U	73	GLY	2.3
1	X	2044	G	2.3
3	A	163	SER	2.3
1	X	1093	U	2.3
12	J	21	ASP	2.3
5	C	172	VAL	2.2
1	X	1074	G	2.2
21	S	69	VAL	2.2
26	Z	5	PRO	2.2
9	G	167	LYS	2.2
11	I	100	ARG	2.2
20	R	113	THR	2.2
1	X	1553	G	2.2
21	S	123	VAL	2.2
1	X	1099	A	2.2
1	X	1841	G	2.2
11	I	24	GLY	2.2
21	S	58	GLY	2.2
24	V	65	GLU	2.2
6	D	136	LEU	2.2
28	2	38	GLY	2.2
20	R	83	LEU	2.2
8	F	109	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
28	2	39	ARG	2.2
25	W	54	GLN	2.2
7	E	174	GLY	2.2
8	F	100	ASN	2.2
21	S	114	ASP	2.2
1	X	1551	U	2.1
20	R	95	ARG	2.1
9	G	66	HIS	2.1
14	L	58	ALA	2.1
3	A	92	ARG	2.1
3	A	272	VAL	2.1
14	L	34	SER	2.1
20	R	103	LYS	2.1
23	U	57	VAL	2.1
29	3	20	GLY	2.1
12	J	72	ASP	2.1
7	E	68	THR	2.1
7	E	82	GLY	2.1
23	U	50	ALA	2.1
11	I	50	GLU	2.1
19	Q	65	VAL	2.1
16	N	23	GLY	2.1
22	T	61	ALA	2.1
5	C	164	VAL	2.1
8	F	79	ARG	2.1
11	I	53	ARG	2.1
16	N	89	ASP	2.1
1	X	1019	U	2.1
1	X	1116	U	2.1
1	X	2169	A	2.1
5	C	21	GLU	2.1
20	R	29	HIS	2.1
6	D	151	GLY	2.1
6	D	11	GLN	2.1
1	X	871	U	2.1
14	L	107	ALA	2.1
1	X	1094	C	2.1
27	1	50	PHE	2.0
6	D	90	THR	2.0
23	U	65	ASN	2.0
1	X	69	G	2.0
30	4	31	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
28	2	46	ASP	2.0
8	F	130	THR	2.0
15	M	28	ARG	2.0
29	3	25	PHE	2.0
1	X	1073	G	2.0
1	X	1121	G	2.0
1	X	1556	A	2.0
1	X	2299	A	2.0
23	U	49	LYS	2.0
20	R	99	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
33	NA	X	3064	1/1	0.72	0.27	58,58,58,58	0
34	K	X	3074	1/1	0.75	0.67	171,171,171,171	0
34	K	X	3076	1/1	0.76	0.36	100,100,100,100	0
32	MG	X	2891	1/1	0.78	0.20	56,56,56,56	0
33	NA	Y	126	1/1	0.80	0.40	85,85,85,85	0
33	NA	X	3061	1/1	0.81	0.55	62,62,62,62	0
32	MG	X	2939	1/1	0.83	0.56	79,79,79,79	0
33	NA	X	3037	1/1	0.83	0.26	53,53,53,53	0
33	NA	A	277	1/1	0.83	0.43	72,72,72,72	0
33	NA	X	3053	1/1	0.83	0.53	62,62,62,62	0
32	MG	X	2931	1/1	0.83	0.59	48,48,48,48	0
32	MG	X	2992	1/1	0.84	0.23	44,44,44,44	0
33	NA	X	3069	1/1	0.84	0.94	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	X	3023	1/1	0.85	0.32	73,73,73,73	0
32	MG	X	2975	1/1	0.86	0.23	73,73,73,73	0
32	MG	X	2903	1/1	0.86	0.45	51,51,51,51	0
32	MG	X	2952	1/1	0.86	0.44	57,57,57,57	0
32	MG	X	2901	1/1	0.87	0.49	30,30,30,30	0
32	MG	X	2966	1/1	0.87	0.29	60,60,60,60	0
32	MG	X	2937	1/1	0.88	0.24	46,46,46,46	0
32	MG	I	157	1/1	0.88	0.35	50,50,50,50	0
33	NA	X	3036	1/1	0.88	0.26	79,79,79,79	0
32	MG	X	2970	1/1	0.88	0.21	51,51,51,51	0
32	MG	X	2997	1/1	0.88	0.20	50,50,50,50	0
32	MG	X	3015	1/1	0.88	0.45	77,77,77,77	0
33	NA	X	3058	1/1	0.89	0.35	69,69,69,69	0
32	MG	X	2928	1/1	0.89	0.40	41,41,41,41	0
33	NA	X	3046	1/1	0.89	0.59	80,80,80,80	0
32	MG	X	2978	1/1	0.89	0.42	48,48,48,48	0
32	MG	X	2934	1/1	0.90	0.20	62,62,62,62	0
32	MG	X	2918	1/1	0.90	0.21	60,60,60,60	0
32	MG	X	3000	1/1	0.90	0.25	65,65,65,65	0
33	NA	X	3038	1/1	0.90	0.39	59,59,59,59	0
32	MG	X	3004	1/1	0.90	0.39	71,71,71,71	0
33	NA	K	117	1/1	0.90	0.16	28,28,28,28	0
32	MG	X	2887	1/1	0.90	0.31	37,37,37,37	0
31	LMA	X	2881	58/58	0.90	0.27	22,83,114,128	0
32	MG	X	3014	1/1	0.91	0.36	54,54,54,54	0
33	NA	X	3067	1/1	0.91	0.29	47,47,47,47	0
33	NA	X	3050	1/1	0.91	0.30	40,40,40,40	0
32	MG	X	2894	1/1	0.91	0.24	33,33,33,33	0
33	NA	X	3057	1/1	0.91	0.89	75,75,75,75	0
32	MG	X	3019	1/1	0.91	0.41	74,74,74,74	0
34	K	X	3070	1/1	0.91	0.53	72,72,72,72	0
32	MG	X	2988	1/1	0.91	0.29	63,63,63,63	0
33	NA	X	3063	1/1	0.91	0.38	50,50,50,50	0
32	MG	X	2985	1/1	0.92	0.17	50,50,50,50	0
32	MG	X	3022	1/1	0.92	0.14	43,43,43,43	0
32	MG	X	2916	1/1	0.92	0.30	51,51,51,51	0
32	MG	X	2961	1/1	0.92	0.36	61,61,61,61	0
33	NA	X	3066	1/1	0.92	0.42	48,48,48,48	0
32	MG	X	2883	1/1	0.92	0.33	34,34,34,34	0
32	MG	X	2923	1/1	0.92	0.52	66,66,66,66	0
32	MG	X	2910	1/1	0.92	0.29	47,47,47,47	0
32	MG	X	3010	1/1	0.92	0.43	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	X	2940	1/1	0.92	0.25	34,34,34,34	0
33	NA	X	3052	1/1	0.92	0.25	43,43,43,43	0
32	MG	X	2979	1/1	0.92	0.60	50,50,50,50	0
32	MG	X	3018	1/1	0.92	0.40	59,59,59,59	0
32	MG	X	2925	1/1	0.93	0.35	72,72,72,72	0
33	NA	X	3056	1/1	0.93	0.70	76,76,76,76	0
32	MG	X	2914	1/1	0.93	0.61	60,60,60,60	0
32	MG	X	2930	1/1	0.93	0.53	51,51,51,51	0
32	MG	X	3027	1/1	0.93	0.17	51,51,51,51	0
33	NA	X	3062	1/1	0.93	0.14	47,47,47,47	0
32	MG	X	3028	1/1	0.93	0.18	65,65,65,65	0
32	MG	X	3032	1/1	0.93	0.37	74,74,74,74	0
32	MG	X	2968	1/1	0.93	0.26	56,56,56,56	0
32	MG	X	2907	1/1	0.93	0.48	66,66,66,66	0
32	MG	X	3007	1/1	0.93	0.20	37,37,37,37	0
32	MG	X	2942	1/1	0.93	0.20	74,74,74,74	0
33	NA	X	3039	1/1	0.93	0.28	51,51,51,51	0
32	MG	X	2945	1/1	0.93	0.46	32,32,32,32	0
33	NA	X	3049	1/1	0.93	0.49	68,68,68,68	0
32	MG	X	2949	1/1	0.93	0.41	48,48,48,48	0
32	MG	X	2950	1/1	0.93	0.25	49,49,49,49	0
34	K	X	3077	1/1	0.93	0.45	80,80,80,80	0
34	K	X	3079	1/1	0.93	0.47	97,97,97,97	0
32	MG	X	2984	1/1	0.94	0.29	62,62,62,62	0
32	MG	X	2957	1/1	0.94	0.40	35,35,35,35	0
32	MG	X	2987	1/1	0.94	0.46	38,38,38,38	0
32	MG	X	2921	1/1	0.94	0.23	52,52,52,52	0
32	MG	X	2963	1/1	0.94	0.27	69,69,69,69	0
32	MG	X	3029	1/1	0.94	0.41	63,63,63,63	0
32	MG	X	2995	1/1	0.94	0.63	42,42,42,42	0
32	MG	X	2943	1/1	0.94	0.52	29,29,29,29	0
33	NA	X	3035	1/1	0.94	0.30	50,50,50,50	0
32	MG	X	2999	1/1	0.94	0.18	49,49,49,49	0
32	MG	X	2911	1/1	0.94	0.47	83,83,83,83	0
32	MG	X	2969	1/1	0.94	0.24	31,31,31,31	0
32	MG	X	2908	1/1	0.94	0.32	55,55,55,55	0
33	NA	X	3044	1/1	0.94	0.09	48,48,48,48	0
33	NA	Z	61	1/1	0.94	0.30	48,48,48,48	0
32	MG	X	2972	1/1	0.94	0.21	65,65,65,65	0
33	NA	X	3047	1/1	0.94	0.59	75,75,75,75	0
32	MG	X	2909	1/1	0.94	0.43	44,44,44,44	0
32	MG	X	2895	1/1	0.94	0.35	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	X	2953	1/1	0.94	0.21	59,59,59,59	0
34	K	X	3082	1/1	0.94	0.29	98,98,98,98	0
32	MG	X	2885	1/1	0.95	0.50	21,21,21,21	0
32	MG	X	2912	1/1	0.95	0.34	24,24,24,24	0
32	MG	X	2989	1/1	0.95	0.40	83,83,83,83	0
33	NA	X	3055	1/1	0.95	0.28	70,70,70,70	0
32	MG	X	2922	1/1	0.95	0.18	19,19,19,19	0
32	MG	X	3024	1/1	0.95	0.28	68,68,68,68	0
32	MG	X	3026	1/1	0.95	0.33	37,37,37,37	0
33	NA	X	3059	1/1	0.95	0.13	66,66,66,66	0
32	MG	X	2993	1/1	0.95	0.36	51,51,51,51	0
32	MG	X	2935	1/1	0.95	0.32	55,55,55,55	0
32	MG	X	2936	1/1	0.95	0.27	26,26,26,26	0
32	MG	X	3030	1/1	0.95	0.10	66,66,66,66	0
32	MG	X	2913	1/1	0.95	0.43	56,56,56,56	0
32	MG	X	2893	1/1	0.95	0.48	25,25,25,25	0
32	MG	X	3002	1/1	0.95	0.22	34,34,34,34	0
32	MG	X	3003	1/1	0.95	0.48	55,55,55,55	0
32	MG	X	2956	1/1	0.95	0.66	71,71,71,71	0
32	MG	X	3005	1/1	0.95	0.15	58,58,58,58	0
32	MG	X	2900	1/1	0.95	0.41	37,37,37,37	0
33	NA	X	3042	1/1	0.95	0.48	45,45,45,45	0
34	K	X	3072	1/1	0.95	0.21	104,104,104,104	0
32	MG	X	3008	1/1	0.95	0.25	45,45,45,45	0
34	K	X	3075	1/1	0.95	0.22	68,68,68,68	0
32	MG	X	2983	1/1	0.95	0.26	23,23,23,23	0
32	MG	X	2960	1/1	0.95	0.36	33,33,33,33	0
34	K	X	3078	1/1	0.95	0.32	91,91,91,91	0
33	NA	X	3048	1/1	0.95	0.26	71,71,71,71	0
32	MG	X	2941	1/1	0.95	0.43	46,46,46,46	0
32	MG	X	2982	1/1	0.96	0.48	51,51,51,51	0
32	MG	X	2964	1/1	0.96	0.44	50,50,50,50	0
32	MG	Y	124	1/1	0.96	0.11	40,40,40,40	0
32	MG	X	2892	1/1	0.96	0.22	30,30,30,30	0
33	NA	X	3034	1/1	0.96	0.31	50,50,50,50	0
32	MG	X	2919	1/1	0.96	0.35	61,61,61,61	0
32	MG	X	2944	1/1	0.96	0.35	59,59,59,59	0
33	NA	X	3065	1/1	0.96	0.38	58,58,58,58	0
32	MG	X	2933	1/1	0.96	0.49	59,59,59,59	0
32	MG	X	3012	1/1	0.96	0.57	45,45,45,45	0
32	MG	X	2971	1/1	0.96	0.24	44,44,44,44	0
33	NA	X	3041	1/1	0.96	0.30	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	X	2990	1/1	0.96	0.39	31,31,31,31	0
32	MG	X	2947	1/1	0.96	0.39	47,47,47,47	0
32	MG	X	2974	1/1	0.96	0.18	37,37,37,37	0
32	MG	X	3021	1/1	0.96	0.54	70,70,70,70	0
34	K	X	3071	1/1	0.96	0.23	86,86,86,86	0
32	MG	X	2994	1/1	0.96	0.10	41,41,41,41	0
32	MG	X	2920	1/1	0.96	0.36	31,31,31,31	0
32	MG	X	2976	1/1	0.96	0.24	32,32,32,32	0
33	NA	X	3051	1/1	0.96	0.24	43,43,43,43	0
32	MG	X	2998	1/1	0.96	0.38	29,29,29,29	0
32	MG	X	2977	1/1	0.96	0.32	51,51,51,51	0
32	MG	X	2962	1/1	0.96	0.13	70,70,70,70	0
32	MG	X	2897	1/1	0.96	0.36	37,37,37,37	0
34	K	X	3083	1/1	0.96	0.28	103,103,103,103	0
32	MG	X	3009	1/1	0.97	0.24	53,53,53,53	0
32	MG	X	2882	1/1	0.97	0.33	5,5,5,5	0
33	NA	X	3033	1/1	0.97	0.44	38,38,38,38	0
32	MG	X	3011	1/1	0.97	0.55	45,45,45,45	0
32	MG	X	2884	1/1	0.97	0.54	38,38,38,38	0
32	MG	X	3013	1/1	0.97	0.11	60,60,60,60	0
32	MG	X	2958	1/1	0.97	0.10	29,29,29,29	0
32	MG	X	2902	1/1	0.97	0.35	39,39,39,39	0
32	MG	X	3016	1/1	0.97	0.35	39,39,39,39	0
32	MG	X	3017	1/1	0.97	0.51	70,70,70,70	0
33	NA	Y	125	1/1	0.97	0.44	62,62,62,62	0
32	MG	X	2889	1/1	0.97	0.26	26,26,26,26	0
33	NA	X	3043	1/1	0.97	0.31	48,48,48,48	0
32	MG	X	2905	1/1	0.97	0.37	57,57,57,57	0
32	MG	X	3020	1/1	0.97	0.35	42,42,42,42	0
32	MG	X	2906	1/1	0.97	0.39	43,43,43,43	0
32	MG	X	2981	1/1	0.97	0.47	65,65,65,65	0
32	MG	X	2948	1/1	0.97	0.43	40,40,40,40	0
34	K	X	3073	1/1	0.97	0.39	57,57,57,57	0
32	MG	X	3001	1/1	0.97	0.46	84,84,84,84	0
32	MG	X	2965	1/1	0.97	0.31	42,42,42,42	0
32	MG	X	2899	1/1	0.97	0.30	57,57,57,57	0
32	MG	X	2915	1/1	0.97	0.55	47,47,47,47	0
33	NA	X	3054	1/1	0.97	0.38	49,49,49,49	0
32	MG	X	2926	1/1	0.97	0.17	35,35,35,35	0
34	K	X	3080	1/1	0.97	0.49	94,94,94,94	0
34	K	X	3081	1/1	0.97	0.36	91,91,91,91	0
32	MG	X	2927	1/1	0.97	0.21	55,55,55,55	0

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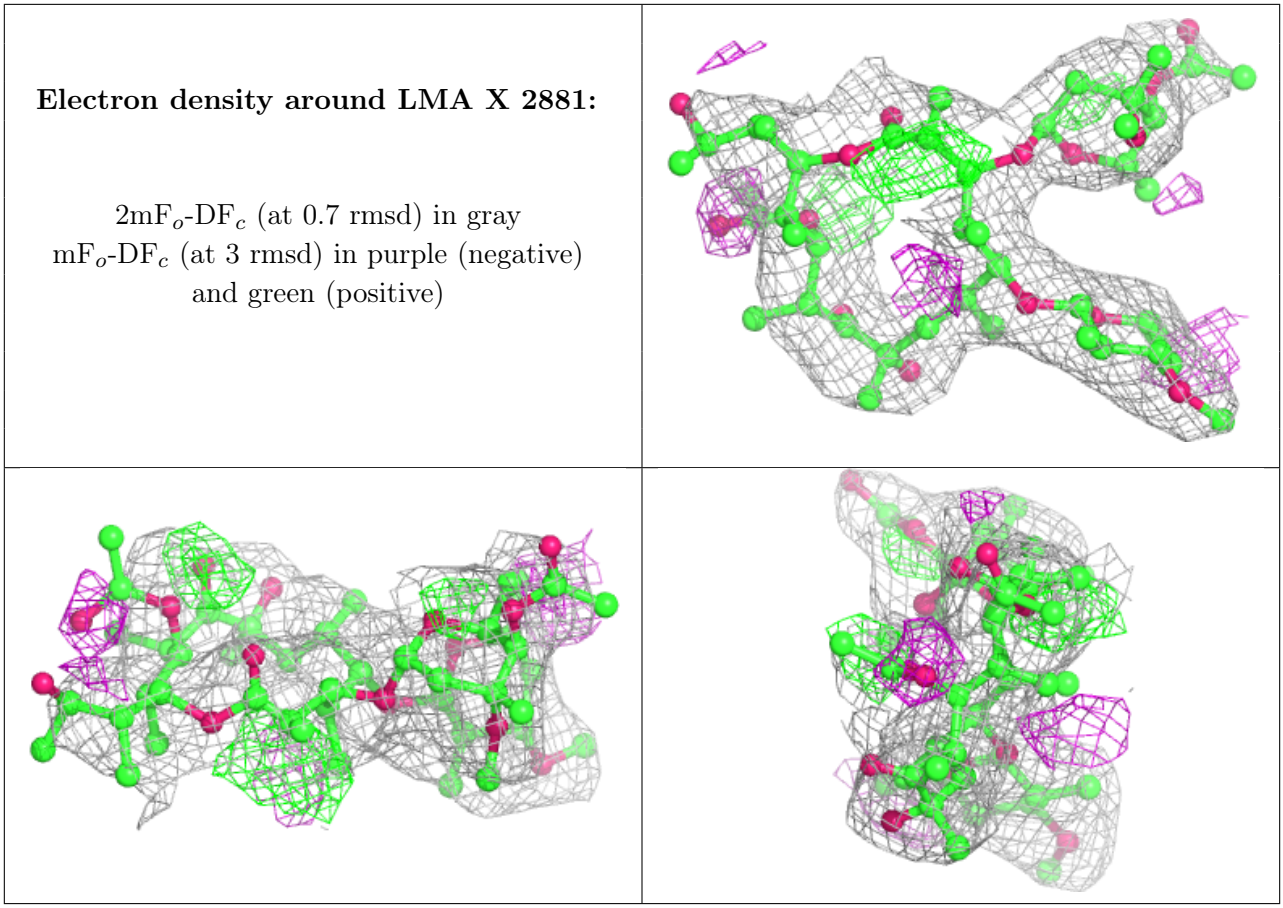
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	X	2955	1/1	0.97	0.37	54,54,54,54	0
34	K	M	167	1/1	0.97	0.38	44,44,44,44	0
33	NA	X	3068	1/1	0.98	0.31	64,64,64,64	0
32	MG	X	2973	1/1	0.98	0.22	30,30,30,30	0
32	MG	X	3031	1/1	0.98	0.15	48,48,48,48	0
32	MG	X	2986	1/1	0.98	0.26	54,54,54,54	0
32	MG	X	2954	1/1	0.98	0.30	31,31,31,31	0
32	MG	C	206	1/1	0.98	0.20	37,37,37,37	0
32	MG	X	2946	1/1	0.98	0.45	38,38,38,38	0
32	MG	X	2886	1/1	0.98	0.36	16,16,16,16	0
32	MG	X	2888	1/1	0.98	0.46	36,36,36,36	0
32	MG	X	2991	1/1	0.98	0.38	51,51,51,51	0
32	MG	X	3006	1/1	0.98	0.07	59,59,59,59	0
32	MG	X	2967	1/1	0.98	0.31	50,50,50,50	0
32	MG	X	2924	1/1	0.98	0.31	26,26,26,26	0
32	MG	X	2959	1/1	0.98	0.40	33,33,33,33	0
33	NA	X	3060	1/1	0.98	0.70	73,73,73,73	0
33	NA	X	3040	1/1	0.98	0.41	70,70,70,70	0
32	MG	X	3025	1/1	0.98	0.19	62,62,62,62	0
32	MG	X	2896	1/1	0.98	0.41	28,28,28,28	0
32	MG	X	2996	1/1	0.98	0.08	42,42,42,42	0
32	MG	X	2938	1/1	0.98	0.40	34,34,34,34	0
33	NA	X	3045	1/1	0.98	0.45	31,31,31,31	0
32	MG	X	2904	1/1	0.98	0.49	39,39,39,39	0
32	MG	X	2917	1/1	0.99	0.27	52,52,52,52	0
32	MG	X	2951	1/1	0.99	0.36	28,28,28,28	0
32	MG	X	2890	1/1	0.99	0.24	38,38,38,38	0
32	MG	X	2932	1/1	0.99	0.36	31,31,31,31	0
32	MG	X	2898	1/1	0.99	0.39	8,8,8,8	0
32	MG	X	2929	1/1	0.99	0.32	10,10,10,10	0
32	MG	X	2980	1/1	0.99	0.12	42,42,42,42	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 LMA X 2881:

$2mF_o$-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.