



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:28 PM UTC

PDB ID : 3PIO / pdb_00003pio
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

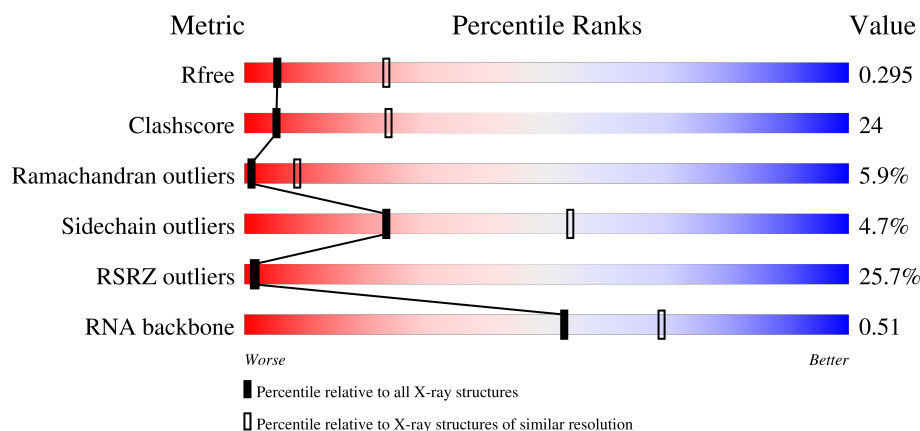
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)
RNA backbone	3983	1047 (3.52-2.96)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	2880	
2	Y	123	
3	A	274	

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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
32	MG	X	2988	-	-	-	X
33	NA	X	3046	-	-	-	X
33	NA	X	3048	-	-	-	X
33	NA	X	3055	-	-	-	X
33	NA	Y	126	-	-	-	X
34	K	X	3074	-	-	-	X

2 Entry composition

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
1	X	2657	Total	C	N	O	P	0	0	0
			57035	25441	10530	18408	2656			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0	0
			2561	1143	471	827	120			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	253	Total	C	N	O	S	0	0	0
			1920	1196	382	340	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	194	Total	C	N	O	S	0	0	0
			1481	920	284	275	2			

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

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

- 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	S	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	C	N	O	0	0	0
			779	476	161	142			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	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			

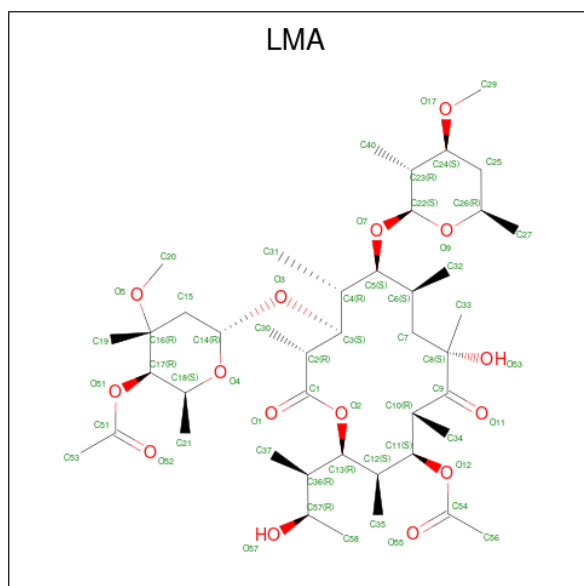
- Molecule 29 is a protein called 50S ribosomal protein L35.

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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

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

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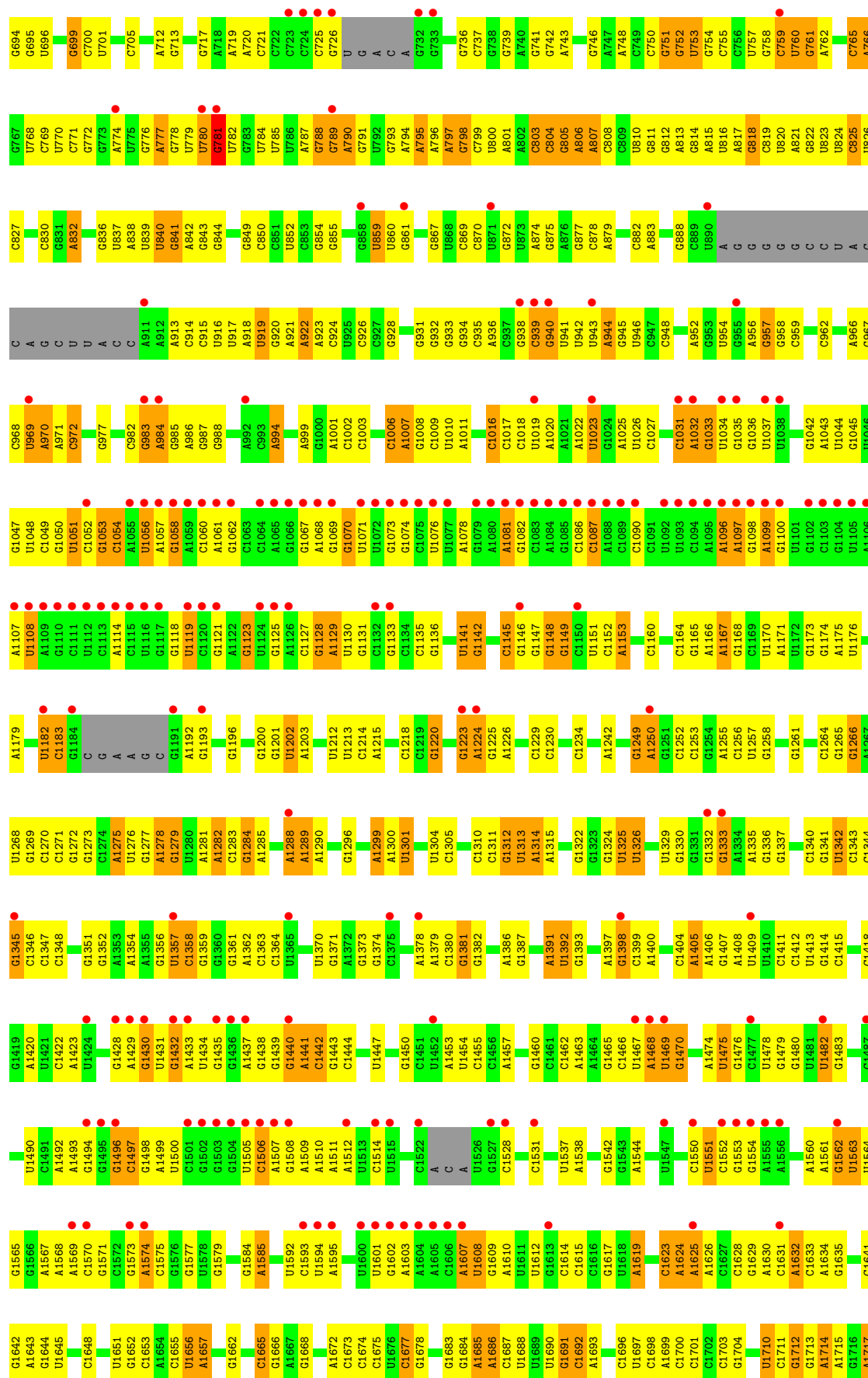
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	Y	1	Total 1	Mg 1	0	0
32	C	1	Total 1	Mg 1	0	0
32	I	1	Total 1	Mg 1	0	0

- Molecule 33 is SODIUM ION (CCD ID: NA) (formula: Na).

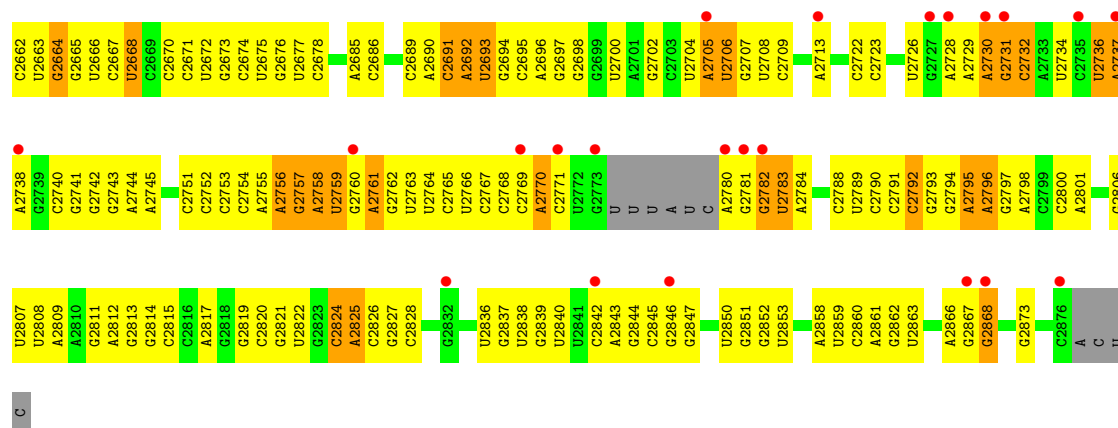
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	37	Total 37	Na 37	0	0
33	Y	2	Total 2	Na 2	0	0
33	A	1	Total 1	Na 1	0	0
33	K	1	Total 1	Na 1	0	0
33	Z	1	Total 1	Na 1	0	0

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

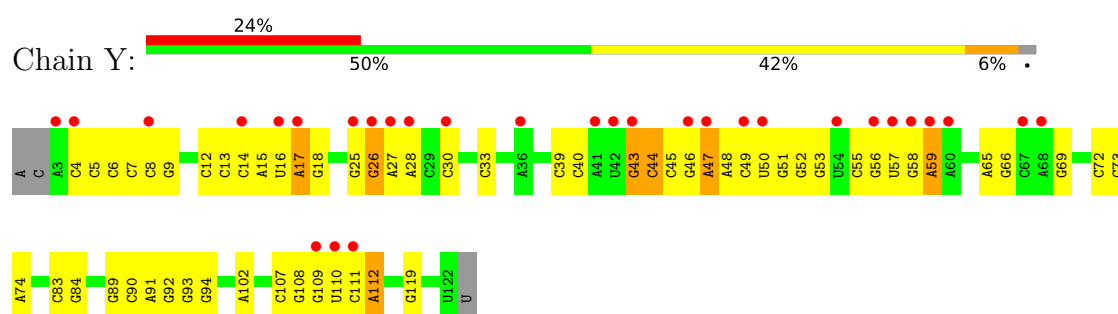
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	X	14	Total 14	K 14	0	0
34	M	1	Total 1	K 1	0	0



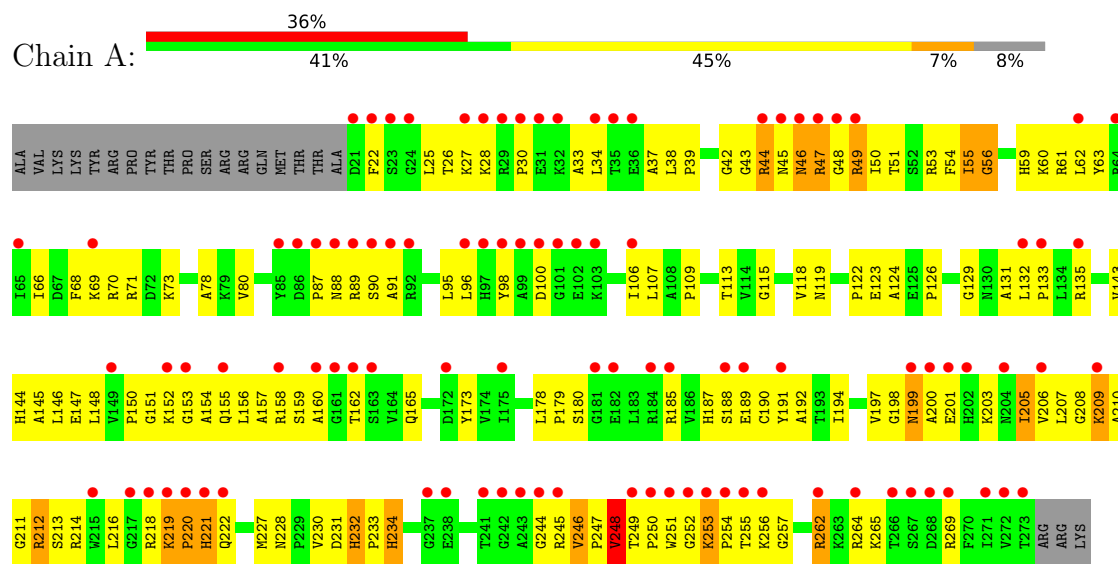




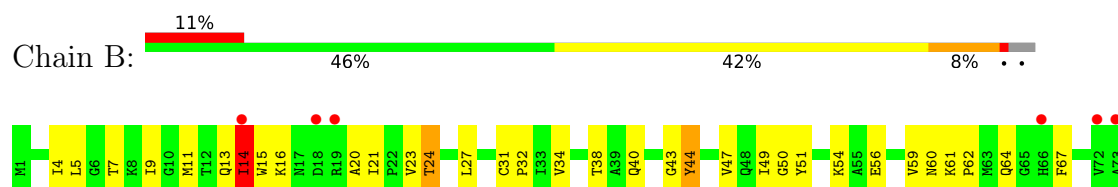
• Molecule 2: 5S ribosomal RNA

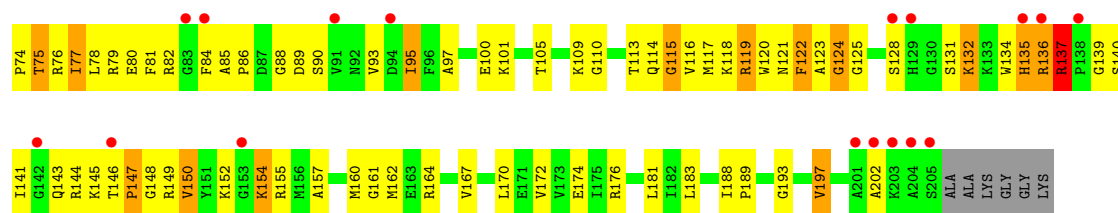


• Molecule 3: 50S ribosomal protein L2



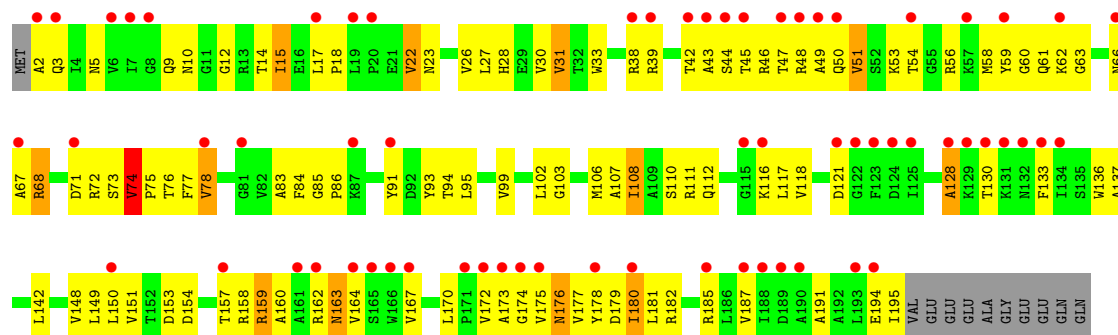
• Molecule 4: 50S ribosomal protein L3





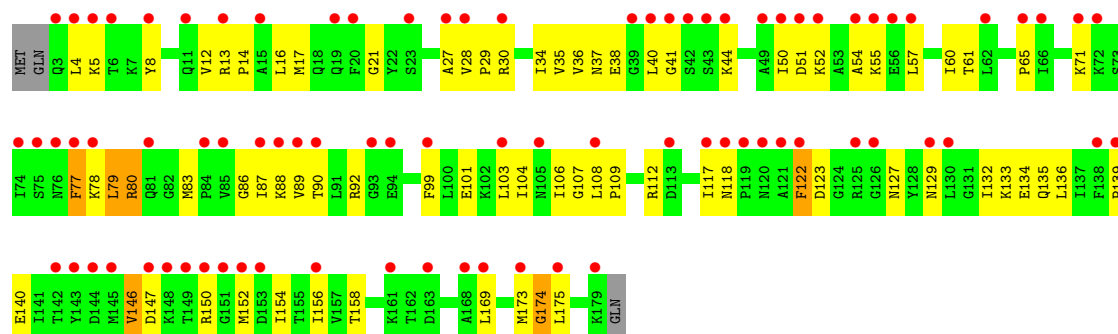
• Molecule 5: 50S ribosomal protein L4

Chain C: 32% 42% 46% 6% 5%



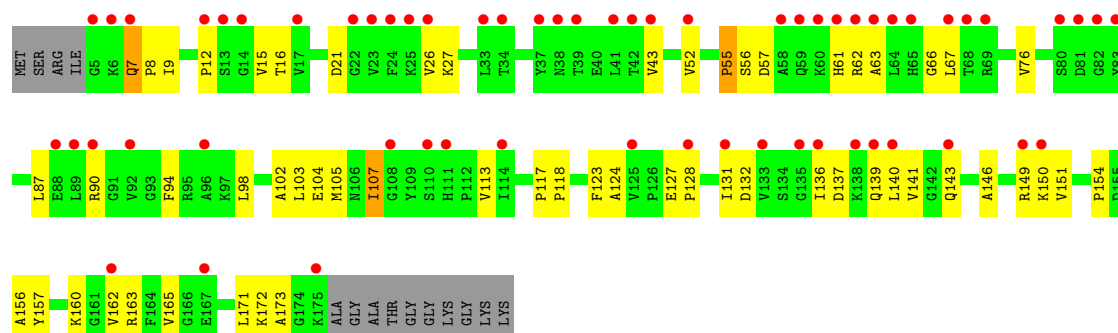
• Molecule 6: 50S ribosomal protein L5

Chain D: 46% 57% 38% 2%

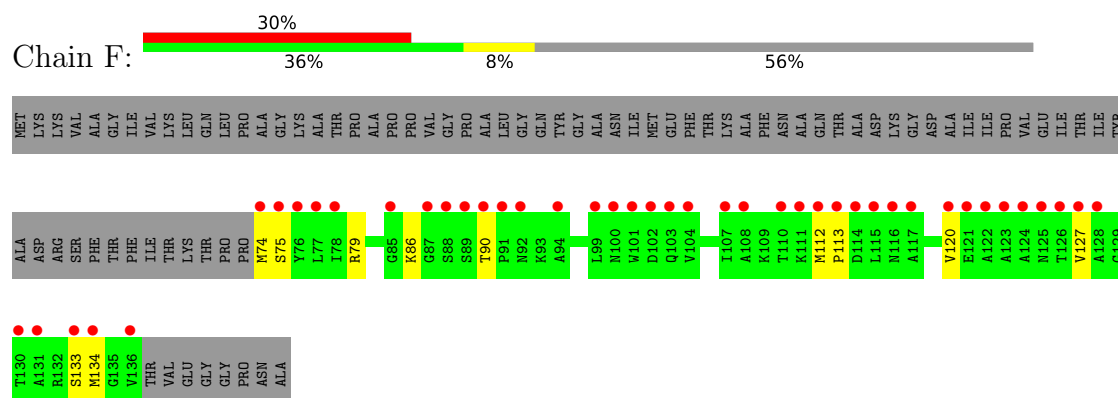


• Molecule 7: 50S ribosomal protein L6

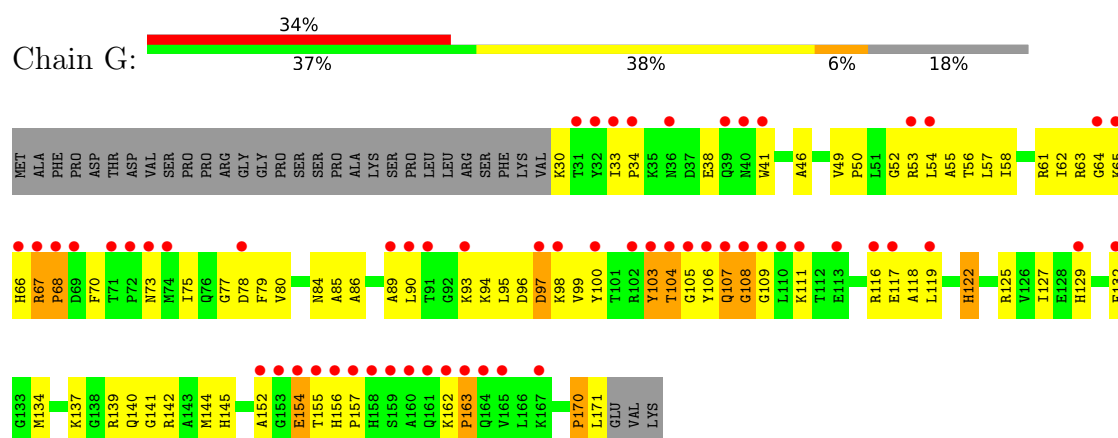
Chain E: 32% 61% 30% 8%



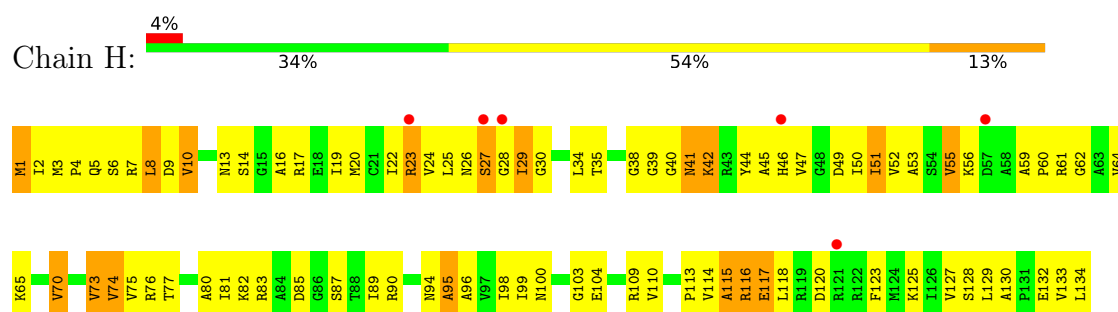
- Molecule 8: 50S ribosomal protein L11



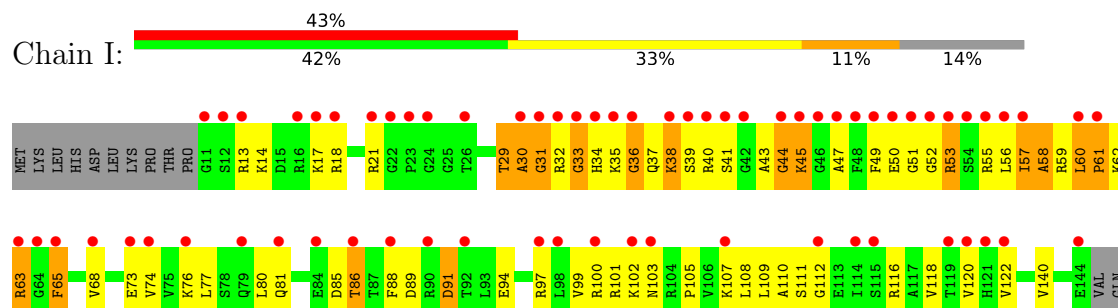
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14



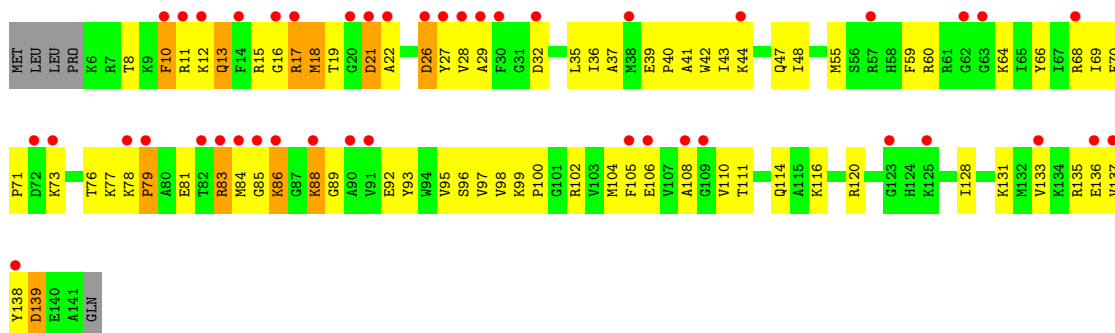
- Molecule 11: 50S ribosomal protein L15



THR
GLN
GLN
ASP
ALA
GLN
LYS
ALA
GLU

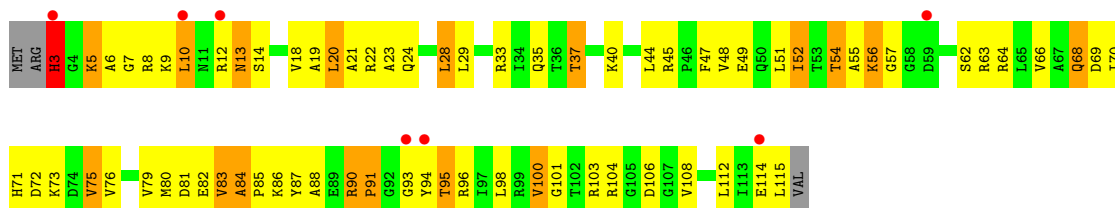
• Molecule 12: 50S ribosomal protein L16

Chain J: 



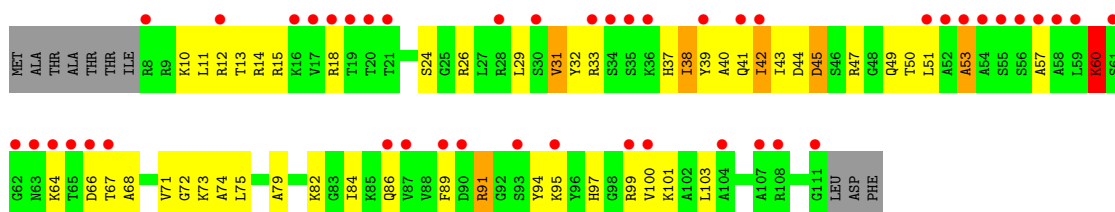
• Molecule 13: 50S ribosomal protein L17

Chain K: 



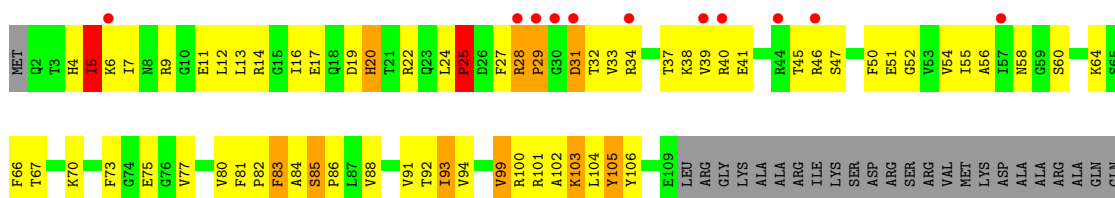
• Molecule 14: 50S ribosomal protein L18

Chain L: 



• Molecule 15: 50S ribosomal protein L19

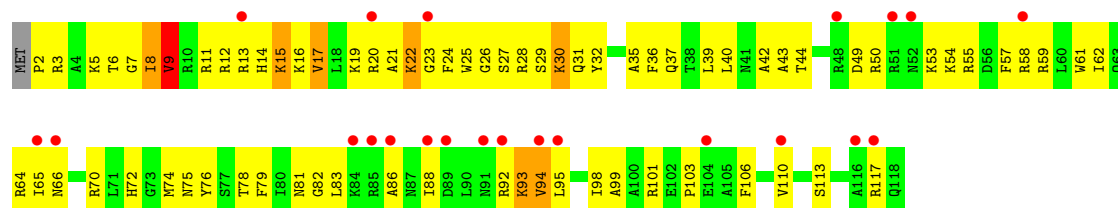
Chain M: 



ASP
LYS
ALA
ASN
ALA
SER
ALA
SER
GLN
ALA
ALA
ALA
GLN
ALA
ASP
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VAL
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ALA
PRO
GLU
VAL
ALA
PRO
THR
GLY
GLU

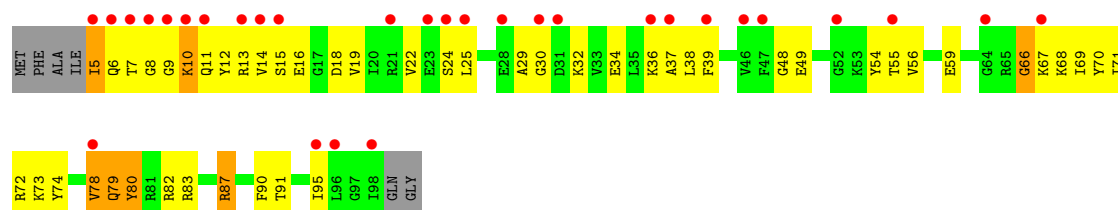
• Molecule 16: 50S ribosomal protein L20

Chain N: 



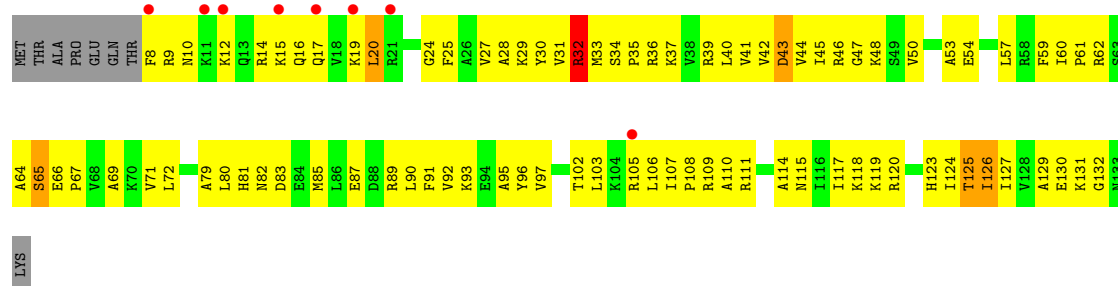
• Molecule 17: 50S ribosomal protein L21

Chain O: 



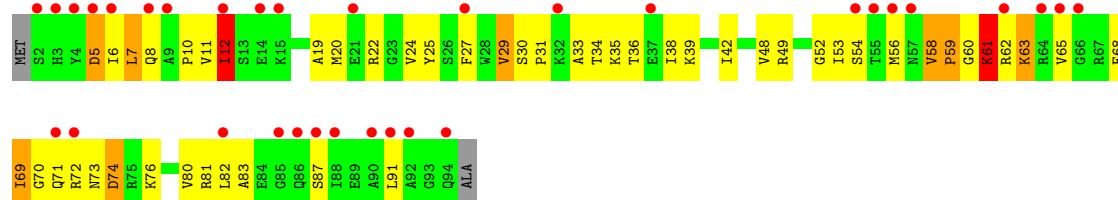
• Molecule 18: 50S ribosomal protein L22

Chain P: 

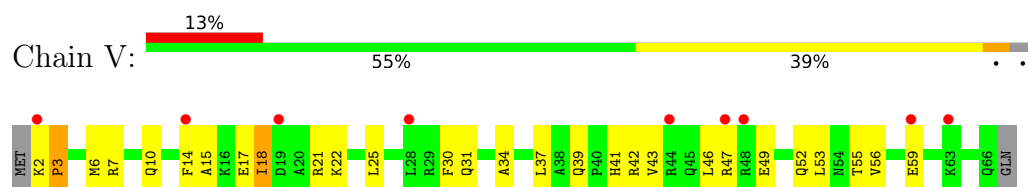


• Molecule 19: 50S ribosomal protein L23

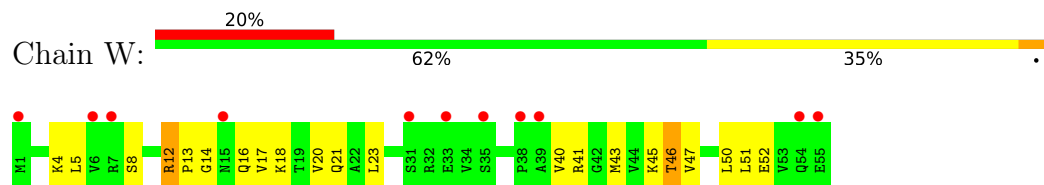
Chain Q: 



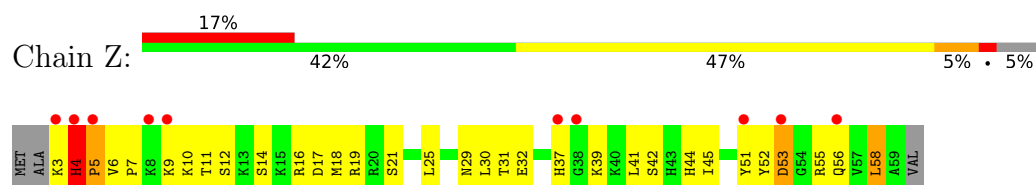
• Molecule 20: 50S ribosomal protein L24



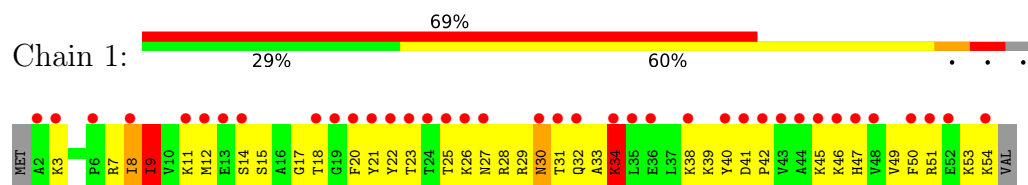
- Molecule 25: 50S ribosomal protein L30



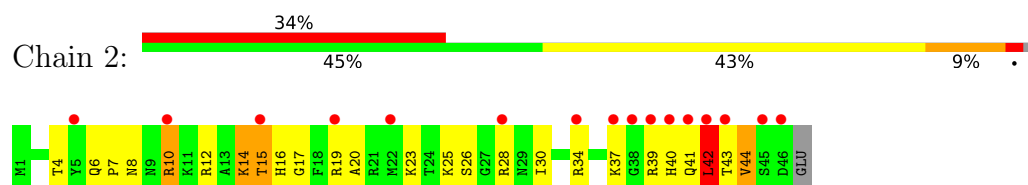
- Molecule 26: 50S ribosomal protein L32



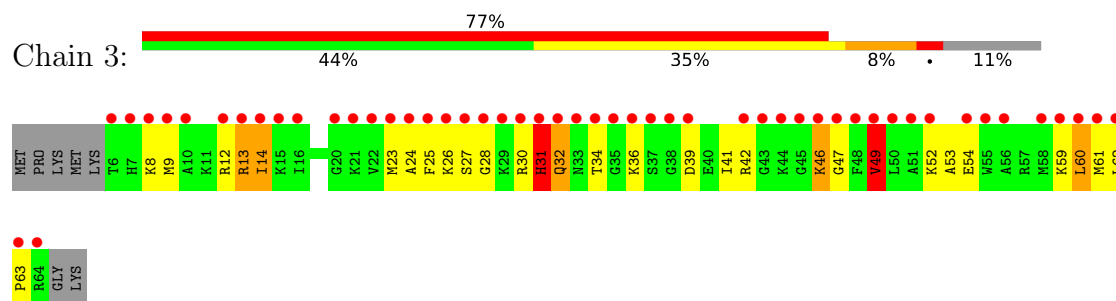
- Molecule 27: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L34

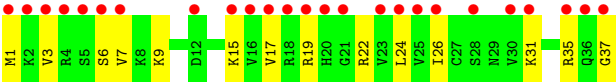


- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.59Å 410.20Å 695.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25 20.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-3.25) 92.9 (20.00-3.25)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.252 , 0.294 0.254 , 0.295	Depositor DCC
R_{free} test set	3594 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)	0.19 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LMA, K, MG, NA

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	0.40	2/63867 (0.0%)	0.45	3/99618 (0.0%)
2	Y	0.27	0/2863	0.33	0/4461
3	A	0.62	0/1958	0.98	8/2638 (0.3%)
4	B	0.73	0/1567	1.09	4/2105 (0.2%)
5	C	0.66	1/1504 (0.1%)	1.05	5/2036 (0.2%)
6	D	0.39	0/1419	0.77	0/1903
7	E	0.45	0/1308	0.86	1/1771 (0.1%)
8	F	0.32	0/455	0.67	0/611
9	G	0.68	0/1138	1.05	3/1539 (0.2%)
10	H	0.83	2/1007 (0.2%)	1.24	5/1352 (0.4%)
11	I	0.70	1/1022 (0.1%)	0.97	1/1366 (0.1%)
12	J	0.61	0/1113	0.99	3/1486 (0.2%)
13	K	1.04	2/886 (0.2%)	1.38	11/1188 (0.9%)
14	L	0.49	0/785	0.80	0/1048
15	M	0.78	0/884	1.23	5/1186 (0.4%)
16	N	0.69	1/994 (0.1%)	1.00	1/1323 (0.1%)
17	O	0.54	0/750	0.93	2/1000 (0.2%)
18	P	0.74	0/1017	1.12	1/1362 (0.1%)
19	Q	0.61	0/737	0.99	4/988 (0.4%)
20	R	0.60	0/835	0.89	0/1121
21	S	0.44	0/1370	0.84	0/1862
22	T	0.51	0/563	0.86	2/747 (0.3%)
23	U	0.55	0/556	0.85	1/741 (0.1%)
24	V	0.39	0/529	0.79	0/704
25	W	0.52	0/426	0.99	2/568 (0.4%)
26	Z	0.77	0/464	1.18	2/622 (0.3%)
27	1	0.56	0/438	0.84	0/583
28	2	0.70	0/387	1.08	3/509 (0.6%)
29	3	0.71	1/468 (0.2%)	0.91	1/614 (0.2%)
30	4	0.34	0/298	0.77	0/390
All	All	0.48	10/91608 (0.0%)	0.63	68/137442 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	29	THR	CA-CB	8.77	1.64	1.53
13	K	52	ILE	CA-CB	7.34	1.62	1.54
13	K	3	HIS	CA-C	6.93	1.67	1.52
10	H	55	VAL	CA-CB	-6.63	1.46	1.54
29	3	49	VAL	CA-CB	-6.20	1.46	1.54
16	N	21	ALA	CA-CB	-5.33	1.46	1.52
5	C	51	VAL	CA-CB	5.17	1.61	1.54
1	X	1333	G	O3'-P	-5.14	1.53	1.61
1	X	1202	U	O3'-P	-5.14	1.53	1.61
10	H	70	VAL	CA-CB	-5.12	1.47	1.55

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	212	ARG	N-CA-C	-10.61	99.60	112.54
12	J	86	LYS	N-CA-C	10.06	117.03	108.78
13	K	83	VAL	N-CA-C	9.54	119.56	110.30
11	I	41	SER	N-CA-C	8.91	123.42	111.30
26	Z	4	HIS	CA-C-N	-8.72	108.93	119.84
26	Z	4	HIS	C-N-CA	-8.72	108.93	119.84
5	C	74	VAL	CA-C-N	8.53	129.37	119.47
5	C	74	VAL	C-N-CA	8.53	129.37	119.47
10	H	117	GLU	N-CA-C	-7.19	103.77	112.54
25	W	12	ARG	CA-C-N	7.09	127.50	119.92
25	W	12	ARG	C-N-CA	7.09	127.50	119.92
19	Q	58	VAL	CA-C-N	6.78	128.31	119.84
19	Q	58	VAL	C-N-CA	6.78	128.31	119.84
4	B	125	GLY	CA-C-N	6.70	126.46	119.76
4	B	125	GLY	C-N-CA	6.70	126.46	119.76
3	A	232	HIS	CA-C-N	6.54	128.01	119.84
3	A	232	HIS	C-N-CA	6.54	128.01	119.84
9	G	103	TYR	N-CA-C	6.51	120.64	110.17
13	K	83	VAL	CB-CA-C	-6.51	103.68	111.81
12	J	85	GLY	N-CA-C	-6.45	105.01	111.85
15	M	58	ASN	N-CA-C	6.31	119.50	110.10
13	K	84	ALA	CA-C-N	6.22	125.71	119.24
13	K	84	ALA	C-N-CA	6.22	125.71	119.24
15	M	103	LYS	N-CA-C	6.20	120.58	111.34
3	A	248	VAL	CG1-CB-CG2	-6.20	97.16	110.80
12	J	41	ALA	N-CA-C	6.10	116.29	108.24
10	H	130	ALA	CA-C-N	6.09	127.45	119.84
10	H	130	ALA	C-N-CA	6.09	127.45	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	93	ILE	CB-CA-C	-6.07	103.26	111.15
15	M	5	ILE	CB-CA-C	-5.95	104.78	111.45
13	K	90	ARG	CA-C-N	5.83	127.13	119.84
13	K	90	ARG	C-N-CA	5.83	127.13	119.84
3	A	205	ILE	CB-CA-C	-5.81	105.64	111.80
13	K	10	LEU	CD1-CG-CD2	-5.77	98.11	110.80
19	Q	61	LYS	N-CA-C	5.76	123.07	110.80
17	O	14	VAL	N-CA-C	5.65	112.26	106.21
13	K	52	ILE	N-CA-CB	5.55	116.67	110.51
13	K	3	HIS	N-CA-C	5.54	126.52	111.00
16	N	9	VAL	CB-CA-C	-5.52	104.91	111.81
3	A	262	ARG	N-CA-C	5.50	115.38	108.45
9	G	122	HIS	CA-C-N	5.49	125.14	119.05
9	G	122	HIS	C-N-CA	5.49	125.14	119.05
22	T	17	ASN	CA-C-N	5.49	125.14	119.05
22	T	17	ASN	C-N-CA	5.49	125.14	119.05
7	E	21	ASP	CB-CA-C	-5.46	110.29	116.63
10	H	39	GLY	N-CA-C	5.45	117.59	112.08
13	K	68	GLN	N-CA-C	-5.45	105.36	112.23
4	B	109	LYS	N-CA-C	-5.38	102.92	110.50
17	O	78	VAL	N-CA-C	-5.36	108.05	113.20
5	C	177	VAL	N-CA-C	5.34	116.71	110.62
3	A	46	ASN	CB-CA-C	-5.34	107.73	114.40
5	C	49	ALA	N-CA-C	-5.34	106.72	113.18
18	P	96	TYR	N-CA-C	5.29	116.56	108.52
1	X	781	G	P-O5'-C5'	-5.25	113.03	120.90
10	H	95	ALA	N-CA-C	5.25	117.16	109.24
1	X	2043	A	C4'-C3'-O3'	-5.21	105.18	113.00
5	C	60	GLY	N-CA-C	5.20	118.61	111.54
28	2	6	GLN	CA-C-N	5.20	126.33	119.84
28	2	6	GLN	C-N-CA	5.20	126.33	119.84
3	A	234	HIS	N-CA-C	5.18	117.00	111.36
4	B	51	TYR	N-CA-C	5.18	116.37	108.30
28	2	14	LYS	N-CA-C	5.13	116.56	111.07
1	X	538	A	C3'-C2'-O2'	5.12	122.28	114.60
15	M	94	VAL	CB-CA-C	-5.08	105.26	111.92
23	U	20	ARG	N-CA-C	5.07	116.85	108.13
13	K	8	ARG	N-CA-C	5.07	116.37	109.18
29	3	49	VAL	N-CA-C	5.02	115.14	108.11
19	Q	12	ILE	N-CA-C	5.00	114.37	106.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57035	0	28741	1815	0
2	Y	2561	0	1306	48	0
3	A	1920	0	1974	184	0
4	B	1539	0	1600	151	0
5	C	1481	0	1504	121	0
6	D	1400	0	1481	65	0
7	E	1286	0	1336	44	0
8	F	451	0	474	7	0
9	G	1114	0	1144	102	0
10	H	997	0	1046	101	0
11	I	1011	0	1047	99	0
12	J	1090	0	1125	81	0
13	K	878	0	930	85	0
14	L	779	0	820	74	0
15	M	871	0	894	101	0
16	N	978	0	1020	85	0
17	O	741	0	756	45	0
18	P	1004	0	1083	93	0
19	Q	726	0	753	52	0
20	R	825	0	881	73	0
21	S	1345	0	1372	46	0
22	T	556	0	579	38	0
23	U	552	0	604	48	0
24	V	525	0	546	28	0
25	W	424	0	470	19	0
26	Z	452	0	457	53	0
27	1	431	0	456	59	0
28	2	383	0	414	52	0
29	3	462	0	506	65	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	A	1	0	0	0	0
33	K	1	0	0	0	0
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	3391	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 (3391) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:C:102:LEU:HD21	5:C:106:MET:HE3	1.53	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
3:A:43:GLY:C	3:A:44:ARG:HH11	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
24:V:6:MET:HE3	24:V:56:VAL:HG21	1.57	0.87
2:Y:59:A:H1'	6:D:27:ALA:HB2	1.56	0.86
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:C:162:ARG:HD2	5:C:162:ARG:C	2.05	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
13:K:28:LEU:C	13:K:28:LEU:HD23	2.08	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:X:168:A:H2'	1:X:169:C:C6	2.19	0.78
3:A:245:ARG:C	3:A:253:LYS:HE2	2.09	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
6:D:152:MET:HE2	6:D:154:ILE:HD11	1.66	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
7:E:105:MET:HE1	7:E:131:ILE:HD11	1.68	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
10:H:116:ARG:HD2	15:M:38:LYS:HZ1	1.52	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
29:3:23:MET:HE1	29:3:46:LYS:HD3	1.69	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:795:A:N1	3:A:227:MET:HE3	2.06	0.71
1:X:504:G:H4'	18:P:27:VAL:CG1	2.21	0.71
6:D:80:ARG:HG3	6:D:83:MET:HE3	1.72	0.71
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
3:A:219:LYS:HD2	3:A:219:LYS:C	2.17	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
28:2:37:LYS:C	28:2:40:HIS:HE1	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
19:Q:7:LEU:HD22	19:Q:7:LEU:C	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
9:G:55:ALA:C	9:G:134:MET:HE1	2.19	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
12:J:40:PRO:HB3	12:J:99:LYS:HZ2	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:120:TRP:CD2	4:B:155:ARG:HD2	2.30	0.66
13:K:72:ASP:CG	13:K:75:VAL:HG23	2.20	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
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
5:C:102:LEU:CD2	5:C:106:MET:HE3	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:C:46:ARG:HB3	5:C:51:VAL:HG23	1.79	0.65
9:G:89:ALA:C	9:G:90:LEU:HD12	2.22	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
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
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
4:B:134:TRP:O	4:B:135:HIS:C	2.40	0.65
19:Q:22:ARG:NH1	19:Q:24:VAL:HG21	2.12	0.65
29:3:31:HIS:O	29:3:32:GLN:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
18:P:106:LEU:HD23	18:P:106:LEU:C	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:B:176:ARG:HE	15:M:16:ILE:HG12	1.63	0.63
10:H:42:LYS:HZ2	10:H:46:HIS:HD2	1.45	0.63
9:G:132:PHE:HD2	9:G:145:HIS:CG	2.16	0.63
1:X:795:A:C2	3:A:227:MET:HE3	2.32	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
10:H:1:MET:H3	10:H:1:MET:HE2	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:N:74:MET:HE3	16:N:78:THR:HG22	1.81	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:43:GLY:C	3:A:44:ARG:NH1	2.55	0.62
4:B:147:PRO:O	4:B:149:ARG:N	2.33	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
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
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
28:2:25:LYS:HZ3	28:2:28:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1016:C:HO2'	1:X:1023:U:H5	1.46	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
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
1:X:2662:C:O2	10:H:82:LYS:NZ	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:120:LEU:HD23	21:S:120:LEU:C	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
12:J:40:PRO:CB	12:J:99:LYS:HZ2	2.14	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
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
4:B:93:VAL:C	4:B:95:ILE:H	2.10	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
9:G:117:GLU:C	9:G:119:LEU:H	2.11	0.59
12:J:44:LYS:HD3	12:J:47:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:762:A:H2	1:X:766:A:HO2'	1.48	0.59
3:A:227:MET:HE2	3:A:231:ASP:CB	2.32	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
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
27:1:51:ARG:HD2	27:1:51:ARG:C	2.28	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: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
3:A:227:MET:HE2	3:A:231:ASP:HB3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
24:V:37:LEU:HD23	24:V:37:LEU:C	2.29	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
23:U:21:ARG:C	23:U:39:LYS:HD2	2.28	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
3:A:246:VAL:C	3:A:253:LYS:HD3	2.29	0.58
4:B:121:ASN:O	4:B:122:PHE:C	2.47	0.58
10:H:1:MET:HE2	10:H:1:MET:N	2.19	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
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
13:K:28:LEU:C	13:K:28:LEU:CD2	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:244:GLY:H	3:A:245:ARG:HH11	1.45	0.57
3:A:245:ARG:HA	3:A:253:LYS:HZ1	1.68	0.57
6:D:13:ARG:HG2	6:D:17:MET:HE1	1.85	0.57
13:K:66:VAL:HG21	13:K:80:MET:HE1	1.87	0.57
15:M:67:THR:OG1	15:M:80:VAL:HG22	2.04	0.57
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:247:PRO:C	3:A:249:THR:H	2.12	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
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
15:M:104:LEU:C	15:M:106:TYR:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2670:C:H4'	1:X:2846:G:HO2'	1.71	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
13:K:90:ARG:HG3	13:K:90:ARG:O	2.05	0.56
20:R:93:ARG:O	20:R:94:VAL:C	2.48	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:I:58:ALA:C	11:I:60:LEU:H	2.14	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
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
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:1688:U:O2'	1:X:1690:U:H5	1.90	0.55
1:X:2235:G:N2	1:X:2254:C:N4	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:6:GLN:O	17:O:7:THR:OG1	2.19	0.55
21:S:88:TYR:C	21:S:127:PRO:HG2	2.31	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:26:THR:HG22	3:A:27:LYS:N	2.21	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
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
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
24:V:2:LYS:HA	24:V:6:MET:HE2	1.89	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:C:172:VAL:O	5:C:173:ALA:C	2.50	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
10:H:64:VAL:C	10:H:65:LYS:HD2	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
7:E:105:MET:HE2	7:E:105:MET:HA	1.91	0.53
10:H:65:LYS:HD2	10:H:65:LYS:N	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
19:Q:68:PHE:O	19:Q:69:ILE:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:P:25:PHE:C	18:P:25:PHE:CD2	2.87	0.53
18:P:85:MET:HE3	18:P:130:GLU:HG3	1.90	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
3:A:244:GLY:C	3:A:245:ARG:NE	2.67	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
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:31:GLY:C	11:I:32:ARG:HG3	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
28:2:40:HIS:O	28:2:41:GLN:CD	2.52	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
21:S:13:LYS:HB2	21:S:13:LYS:HZ2	1.73	0.52
27:1:39:LYS:C	27:1:39:LYS:HD3	2.33	0.52
1:X:75:C:N3	1:X:109:A:C2	2.77	0.52
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
20:R:23:ILE:C	20:R:23:ILE:HD12	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:1:MET:HE2	21:S:52:PHE:CD2	2.44	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
15:M:19:ASP:C	15:M:20:HIS:ND1	2.68	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
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
18:P:85:MET:HE1	18:P:129:ALA:HA	1.90	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
1:X:538:A:H3'	9:G:142:ARG:HH22	1.74	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
27:1:39:LYS:HZ3	27:1:41:ASP:HB3	1.74	0.52
1:X:399:G:H4'	23:U:21:ARG:HH12	1.75	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:247:PRO:C	3:A:249:THR:N	2.68	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:22:LYS:C	16:N:24:PHE:H	2.19	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
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:2310:G:O2'	1:X:2315:A:N1	2.38	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
11:I:32:ARG:HH22	17:O:82:ARG:HE	1.58	0.51
16:N:11:ARG:HB3	16:N:15:LYS:HZ1	1.75	0.51
21:S:47:SER:OG	21:S:48:THR:N	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:H:100:ASN:C	10:H:100:ASN:OD1	2.54	0.51
20:R:16:PHE:CZ	20:R:46:VAL:HG22	2.44	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
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
9:G:56:THR:N	9:G:134:MET:HE1	2.25	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
1:X:2757:G:OP2	1:X:2761:A:O2'	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:X:2324:G:HO2'	1:X:2360:C:HO2'	1.46	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:56:LEU:HD22	29:3:52:LYS:NZ	2.26	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
16:N:86:ALA:C	16:N:88:ILE:N	2.69	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
1:X:1300:A:C5'	13:K:103:ARG:HD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:82:ARG:C	4:B:84:PHE:H	2.19	0.50
11:I:56:LEU:HB3	29:3:52:LYS:HZ1	1.76	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
10:H:7:ARG:C	10:H:8:LEU:HD23	2.36	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
1:X:765:C:C5	1:X:1772:C:C2	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1020:A:H4'	16:N:59:ARG:HG3	1.92	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
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
6:D:135:GLN:CD	6:D:150:ARG:H	2.19	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:1947:G:HO2'	1:X:1950:C:P	2.35	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
9:G:84:ASN:C	9:G:86:ALA:H	2.20	0.50
18:P:87:GLU:HA	18:P:90:LEU:CG	2.39	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2722:C:H2'	1:X:2723:C:H6	1.76	0.50
1:X:2796:A:H5''	4:B:162:MET:HE1	1.92	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: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
4:B:14:ILE:CA	15:M:20:HIS:HD2	2.14	0.50
11:I:53:ARG:HD2	11:I:53:ARG:C	2.37	0.50
12:J:35:LEU:HD12	12:J:131:LYS:O	2.11	0.50
23:U:67:LEU:HD23	23:U:67:LEU:C	2.37	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
11:I:45:LYS:C	11:I:45:LYS:HD3	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
24:V:7:ARG:HD2	24:V:7:ARG:C	2.37	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
3:A:122:PRO:HG2	3:A:123:GLU:CD	2.38	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: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
1:X:2262:C:P	27:1:7:ARG:HH22	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:D:51:ASP:O	6:D:55:LYS:HG2	2.12	0.49
20:R:6:ALA:C	20:R:8:SER:H	2.21	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
2:Y:73:C:H2'	2:Y:74:A:O4'	2.12	0.49
5:C:163:ASN:C	5:C:163:ASN:HD22	2.21	0.49
6:D:123:ASP:OD2	6:D:127:ASN:HB2	2.13	0.49
13:K:106:ASP:OD1	13:K:108:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
22:T:12:ASN:C	22:T:14:ARG:H	2.20	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
11:I:43:ALA:O	11:I:44:GLY:C	2.55	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
23:U:59:THR:O	23:U:60:VAL:C	2.56	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
1:X:1911:A:H2'	1:X:1912:G:O4'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
17:O:36:LYS:HZ2	17:O:54:TYR:HB3	1.77	0.48
19:Q:38:ILE:O	19:Q:42:ILE:HG22	2.13	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
3:A:89:ARG:O	3:A:90:SER:C	2.55	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
21:S:127:PRO:C	21:S:129:ARG:H	2.21	0.48
27:1:38:LYS:HD3	27:1:40:TYR:HE1	1.78	0.48
29:3:13:ARG:C	29:3:23:MET:O	2.56	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:1951:G:O2'	1:X:1952:A:O5'	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:86:THR:OG1	11:I:118:VAL:HG12	2.12	0.48
13:K:20:LEU:O	13:K:21:ALA:C	2.55	0.48
14:L:31:VAL:CG2	14:L:33:ARG:HG3	2.44	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:207:LEU:C	3:A:212:ARG:HD3	2.38	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:47:ARG:HD3	3:A:47:ARG:C	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2426:G:C8	1:X:2479:U:C6	3.02	0.48
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
5:C:102:LEU:HD23	5:C:102:LEU:C	2.37	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
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
3:A:46:ASN:O	3:A:47:ARG:C	2.55	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
12:J:21:ASP:C	12:J:99:LYS:HG2	2.38	0.48
16:N:29:SER:C	16:N:30:LYS:HG2	2.38	0.48
16:N:86:ALA:C	16:N:88:ILE:H	2.21	0.48
19:Q:19:ALA:O	19:Q:24:VAL:HB	2.13	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2552:C:H5''	1:X:2553:G:H5''	1.96	0.48
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
9:G:103:TYR:CE1	9:G:111:LYS:C	2.92	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
14:L:42:ILE:HD13	14:L:42:ILE:C	2.39	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
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
20:R:77:HIS:C	20:R:79:SER:H	2.22	0.47
22:T:65:GLY:HA3	22:T:81:ILE:CG2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1979:C:O2	1:X:1980:A:H1'	2.15	0.47
1:X:2324:G:C2	1:X:2360:C:H2'	2.48	0.47
5:C:163:ASN:ND2	5:C:163:ASN:C	2.72	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:1324:G:HO2'	1:X:1325:U:H5	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:P:85:MET:HE2	18:P:130:GLU:HG3	1.97	0.47
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:211:GLY:C	3:A:213:SER:N	2.68	0.47
5:C:102:LEU:HD21	5:C:106:MET:CE	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:20:LEU:O	13:K:22:ARG:N	2.48	0.47
14:L:47:ARG:C	14:L:49:GLN:H	2.23	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
15:M:104:LEU:C	15:M:106:TYR:N	2.73	0.47
16:N:14:HIS:HD2	16:N:32:TYR:CE1	2.33	0.47
16:N:30:LYS:HB3	16:N:30:LYS:HZ2	1.79	0.47
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
29:3:23:MET:HE1	29:3:46:LYS:CD	2.40	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
5:C:62:LYS:HD3	5:C:62:LYS:C	2.39	0.47
7:E:103:LEU:HD12	7:E:104:GLU:N	2.30	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
15:M:82:PRO:C	15:M:84:ALA:N	2.70	0.47
15:M:82:PRO:O	15:M:83:PHE:C	2.58	0.47
26:Z:16:ARG:HD2	26:Z:16:ARG:C	2.40	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:589:C:H4'	16:N:31:GLN:CD	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
21:S:71:MET:N	21:S:71:MET:SD	2.88	0.47
27:1:45:LYS:O	27:1:46:LYS:HB2	2.13	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
9:G:52:GLY:O	9:G:53:ARG:C	2.55	0.46
13:K:98:LEU:CD2	26:Z:56:GLN:HG2	2.41	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
6:D:4:LEU:HD11	6:D:173:MET:HE1	1.97	0.46
9:G:104:THR:H	9:G:107:GLN:HG3	1.79	0.46
11:I:43:ALA:C	11:I:45:LYS:N	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:10:VAL:HG23	10:H:17:ARG:C	2.39	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
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
29:3:53:ALA:O	29:3:54:GLU:C	2.58	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:1782:A:O2'	3:A:208:GLY:O	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:K:18:VAL:O	13:K:19:ALA:C	2.56	0.46
21:S:120:LEU:C	21:S:120:LEU:CD2	2.88	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:59:HIS:O	3:A:60:LYS:C	2.58	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
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
12:J:59:PHE:O	12:J:60:ARG:C	2.59	0.46
15:M:55:ILE:HG22	15:M:104:LEU:HB2	1.98	0.46
20:R:10:HIS:C	20:R:12:ASP:H	2.22	0.46
22:T:69:PHE:C	22:T:70:ILE:HG13	2.40	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
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
5:C:158:ARG:O	5:C:159:ARG:C	2.58	0.46
10:H:2:ILE:HD12	10:H:2:ILE:HG23	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
20:R:22:VAL:HG13	20:R:81:VAL:C	2.38	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
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
5:C:117:LEU:HD23	5:C:117:LEU:C	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:84:ASN:O	9:G:85:ALA:HB3	2.16	0.46
9:G:117:GLU:C	9:G:119:LEU:N	2.69	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: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
1:X:2862:G:H1'	26:Z:29:ASN:HD21	1.81	0.46
3:A:178:LEU:C	3:A:180:SER:H	2.24	0.46
4:B:9:ILE:HD13	15:M:12:LEU:HD13	1.98	0.46
5:C:95:LEU:C	5:C:95:LEU:HD23	2.40	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:72:ASP:OD2	13:K:72:ASP:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
4:B:162:MET:HE2	4:B:162:MET:HB2	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:L:73:LYS:O	14:L:74:ALA:C	2.59	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
14:L:24:SER:C	14:L:26:ARG:H	2.23	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
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
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:O	19:Q:61:LYS:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:LEU:CB	29:3:52:LYS:HZ1	2.29	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
1:X:2299:A:H3'	1:X:2299:A:N3	2.31	0.45
3:A:198:GLY:O	3:A:199:ASN:C	2.58	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: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
17:O:36:LYS:HE3	17:O:55:THR:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1335:A:C2	1:X:1346:C:O2'	2.69	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
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
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:33:ALA:O	3:A:34:LEU:HB3	2.15	0.45
3:A:133:PRO:HD3	3:A:191:TYR:CE2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
10:H:70:VAL:O	10:H:70:VAL:HG13	2.15	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
21:S:1:MET:HE2	21:S:52:PHE:HD2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:93:VAL:C	4:B:95:ILE:N	2.76	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
29:3:36:LYS:HB2	29:3:36:LYS:HE2	1.83	0.44
1:X:54:G:O2'	1:X:125:A:N1	2.49	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
27:1:39:LYS:HZ1	27:1:47:HIS:HA	1.79	0.44
1:X:313:U:O2'	1:X:314:G:H5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
6:D:51:ASP:HA	6:D:54:ALA:HB3	1.99	0.44
7:E:66:GLY:O	7:E:67:LEU:C	2.60	0.44
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
15:M:82:PRO:C	15:M:84:ALA:H	2.26	0.44
20:R:16:PHE:HZ	20:R:46:VAL:CG2	2.31	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:983:G:HO2'	1:X:984:A:P	2.41	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
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
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
9:G:30:LYS:HB2	9:G:30:LYS:HE3	1.68	0.43
9:G:75:ILE:HG22	9:G:144:MET:HE2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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
3:A:256:LYS:O	3:A:257:GLY:C	2.61	0.43
4:B:11:MET:HE2	4:B:11:MET:HB3	1.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:143:GLN:CD	4:B:143:GLN:N	2.76	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
9:G:57:LEU:C	9:G:57:LEU:HD12	2.44	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:1617:G:OP2	19:Q:56:MET:HE1	2.18	0.43
1:X:1947:G:O2'	1:X:1950:C:OP2	2.31	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
6:D:123:ASP:CG	6:D:127:ASN:HB2	2.44	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
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
9:G:61:ARG:HH22	9:G:78:ASP:HB2	1.84	0.43
10:H:26:ASN:O	10:H:27:SER:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:116:ARG:NH1	15:M:38:LYS:HE3	2.33	0.43
14:L:66:ASP:C	14:L:68:ALA:N	2.77	0.43
19:Q:20:MET:HE2	19:Q:20:MET:HB3	1.91	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
1:X:1779:C:C5	1:X:1780:A:N7	2.87	0.43
1:X:2002:A:N7	26:Z:9:LYS:NZ	2.63	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:244:GLY:C	3:A:245:ARG:CZ	2.92	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
3:A:214:ARG:C	3:A:216:LEU:H	2.27	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
10:H:116:ARG:C	10:H:118:LEU:N	2.76	0.42
11:I:77:LEU:HB3	11:I:112:GLY:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
24:V:37:LEU:C	24:V:37:LEU:CD2	2.92	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:555:U:HO2'	1:X:556:A:P	2.42	0.42
1:X:637:G:H8	1:X:637:G:O5'	2.02	0.42
1:X:1290:A:OP1	13:K:40:LYS:NZ	2.52	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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:I:58:ALA:C	11:I:60:LEU:N	2.77	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:42:VAL:O	18:P:43:ASP:C	2.63	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:42:ALA:O	16:N:43:ALA:C	2.62	0.42
20:R:83:LEU:C	20:R:90:LYS:HE2	2.45	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
3:A:227:MET:HE2	3:A:231:ASP:HB2	2.00	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
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:9:LYS:C	13:K:10:LEU:HG	2.44	0.42
13:K:94:TYR:CD2	13:K:115:LEU:O	2.72	0.42
14:L:60:LYS:HG3	14:L:64:LYS:HZ3	1.84	0.42
16:N:14:HIS:CD2	16:N:32:TYR:CE2	3.07	0.42
16:N:57:PHE:O	16:N:58:ARG:C	2.61	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
20:R:85:ASP:C	20:R:87:GLU:H	2.27	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:58:G:H5''	2:Y:59:A:OP1	2.19	0.42
4:B:167:VAL:HG11	4:B:170:LEU:HD21	2.02	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
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
12:J:137:VAL:C	12:J:138:TYR:CD2	2.97	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
1:X:58:C:O2'	1:X:72:A:C8	2.72	0.41
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: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
20:R:75:ALA:C	20:R:76:LEU:HD23	2.45	0.41
26:Z:4:HIS:CD2	26:Z:4:HIS:H	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
1:X:173:A:O2'	1:X:818:G:O6	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:C:172:VAL:O	5:C:172:VAL:HG12	2.19	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
18:P:50:VAL:O	18:P:54:GLU:HG3	2.21	0.41
18:P:106:LEU:C	18:P:106:LEU:CD2	2.93	0.41
1:X:99:U:H3'	1:X:100:G:C5'	2.50	0.41
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:1817:U:H4'	3:A:253:LYS:HZ2	1.85	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:E:103:LEU:HG	7:E:105:MET:HE3	2.01	0.41
12:J:11:ARG:HB3	12:J:12:LYS:H	1.48	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
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: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
3:A:145:ALA:C	3:A:154:ALA:HB1	2.45	0.41
4:B:5:LEU:HD13	4:B:49:ILE:HD13	2.03	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
15:M:102:ALA:C	15:M:103:LYS:HD2	2.46	0.41
20:R:24:VAL:HG11	20:R:28:LYS:O	2.20	0.41
21:S:73:LYS:C	21:S:75:LYS:H	2.29	0.41
24:V:15:ALA:O	24:V:18:ILE:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:J:96:SER:O	12:J:97:VAL:C	2.63	0.41
13:K:22:ARG:O	13:K:23:ALA:C	2.64	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
13:K:66:VAL:CG2	13:K:80:MET:HE1	2.51	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
18:P:71:VAL:O	18:P:72:LEU:C	2.63	0.41
19:Q:62:ARG:HB2	19:Q:63:LYS:H	1.74	0.41
20:R:25:LEU:HD23	20:R:25:LEU:C	2.45	0.41
20:R:48:VAL:C	20:R:50:GLY:H	2.29	0.41
21:S:149:ALA:HB1	21:S:160:LEU:HD13	2.02	0.41
21:S:154:LEU:C	21:S:156:GLU:H	2.29	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:1147:G:C4	1:X:1148:G:C8	3.09	0.41
1:X:1607:A:HO2'	1:X:1608:U:H6	1.68	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:X:1684:G:O2'	1:X:1974:U:O4	2.36	0.40
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:8:C:O2'	14:L:39:TYR:CE1	2.70	0.40
2:Y:26:G:N3	2:Y:58:G:C6	2.90	0.40
3:A:234:HIS:CE1	3:A:253:LYS:HZ3	2.39	0.40
4:B:146:THR:O	4:B:147:PRO:C	2.63	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
13:K:55:ALA:C	13:K:57:GLY:H	2.28	0.40
14:L:66:ASP:C	14:L:68:ALA:H	2.28	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: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: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
10:H:41:ASN:O	10:H:42:LYS:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:C:158:ARG:C	5:C:160:ALA:N	2.78	0.40
9:G:63:ARG:CZ	9:G:144:MET:HE1	2.51	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
13:K:63:ARG:HA	13:K:80:MET:HE3	2.02	0.40
15:M:24:LEU:HD11	15:M:34:ARG:NH2	2.37	0.40
16:N:43:ALA:O	16:N:44:THR:C	2.64	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
25:W:40:VAL:O	25:W:41:ARG:C	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:H:134:LEU:HD23	10:H:134:LEU:HA	1.81	0.40
12:J:55:MET:HE1	12:J:105:PHE:CD1	2.57	0.40
12:J:64:LYS:HZ1	12:J:110:VAL:HG13	1.84	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
25:W:43:MET:HB3	25:W:43:MET:HE3	1.98	0.40
26:Z:3:LYS:C	26:Z:5:PRO:CD	2.95	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	12
4	B	203/211 (96%)	160 (79%)	29 (14%)	14 (7%)	1	6
5	C	192/205 (94%)	143 (74%)	37 (19%)	12 (6%)	1	7
6	D	175/180 (97%)	137 (78%)	32 (18%)	6 (3%)	3	18
7	E	169/185 (91%)	142 (84%)	20 (12%)	7 (4%)	2	14
8	F	61/144 (42%)	48 (79%)	12 (20%)	1 (2%)	7	33
9	G	140/174 (80%)	104 (74%)	27 (19%)	9 (6%)	1	7
10	H	132/134 (98%)	111 (84%)	17 (13%)	4 (3%)	3	20
11	I	132/156 (85%)	82 (62%)	31 (24%)	19 (14%)	0	1
12	J	134/141 (95%)	96 (72%)	27 (20%)	11 (8%)	0	4
13	K	111/116 (96%)	89 (80%)	14 (13%)	8 (7%)	1	5
14	L	102/114 (90%)	73 (72%)	26 (26%)	3 (3%)	3	21
15	M	106/166 (64%)	82 (77%)	18 (17%)	6 (6%)	1	9
16	N	115/118 (98%)	95 (83%)	16 (14%)	4 (4%)	3	17
17	O	92/100 (92%)	68 (74%)	17 (18%)	7 (8%)	1	5
18	P	124/134 (92%)	101 (82%)	18 (14%)	5 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Q	91/95 (96%)	63 (69%)	19 (21%)	9 (10%)	0	2
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	17
22	T	72/91 (79%)	53 (74%)	18 (25%)	1 (1%)	9	35
23	U	70/81 (86%)	50 (71%)	13 (19%)	7 (10%)	0	2
24	V	63/67 (94%)	55 (87%)	5 (8%)	3 (5%)	2	12
25	W	53/55 (96%)	47 (89%)	6 (11%)	0	100	100
26	Z	55/60 (92%)	42 (76%)	9 (16%)	4 (7%)	1	5
27	1	51/55 (93%)	30 (59%)	15 (29%)	6 (12%)	0	1
28	2	44/47 (94%)	37 (84%)	5 (11%)	2 (4%)	2	13
29	3	57/66 (86%)	34 (60%)	18 (32%)	5 (9%)	0	3
30	4	35/37 (95%)	29 (83%)	6 (17%)	0	100	100
All	All	3111/3558 (87%)	2371 (76%)	557 (18%)	183 (6%)	1	9

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	186 (96%)	8 (4%)	27	57
4	B	155/157 (99%)	144 (93%)	11 (7%)	13	42
5	C	154/163 (94%)	147 (96%)	7 (4%)	24	55
6	D	153/156 (98%)	151 (99%)	2 (1%)	61	75
7	E	136/144 (94%)	135 (99%)	1 (1%)	76	81
8	F	46/107 (43%)	46 (100%)	0	100	100
9	G	118/146 (81%)	116 (98%)	2 (2%)	53	72
10	H	103/103 (100%)	93 (90%)	10 (10%)	8	30
11	I	101/121 (84%)	98 (97%)	3 (3%)	36	63
12	J	110/115 (96%)	108 (98%)	2 (2%)	51	71
13	K	90/93 (97%)	80 (89%)	10 (11%)	6	24
14	L	74/82 (90%)	68 (92%)	6 (8%)	11	37
15	M	94/134 (70%)	86 (92%)	8 (8%)	10	34
16	N	96/97 (99%)	89 (93%)	7 (7%)	13	41
17	O	75/79 (95%)	72 (96%)	3 (4%)	28	58
18	P	108/115 (94%)	102 (94%)	6 (6%)	19	49
19	Q	75/76 (99%)	70 (93%)	5 (7%)	15	44
20	R	91/96 (95%)	88 (97%)	3 (3%)	33	62
21	S	149/192 (78%)	147 (99%)	2 (1%)	61	75
22	T	55/67 (82%)	53 (96%)	2 (4%)	31	60
23	U	57/66 (86%)	53 (93%)	4 (7%)	14	42
24	V	53/55 (96%)	53 (100%)	0	100	100
25	W	48/48 (100%)	47 (98%)	1 (2%)	47	69
26	Z	51/53 (96%)	48 (94%)	3 (6%)	18	48
27	1	46/48 (96%)	41 (89%)	5 (11%)	6	25
28	2	39/40 (98%)	35 (90%)	4 (10%)	7	27
29	3	46/52 (88%)	42 (91%)	4 (9%)	9	33
30	4	35/35 (100%)	35 (100%)	0	100	100
All	All	2552/2855 (89%)	2433 (95%)	119 (5%)	23	54

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	44	ARG
3	A	49	ARG
3	A	165	GLN
3	A	199	ASN
3	A	209	LYS
3	A	219	LYS
3	A	246	VAL
3	A	248	VAL
4	B	14	ILE
4	B	24	THR
4	B	44	TYR
4	B	75	THR
4	B	77	ILE
4	B	119	ARG
4	B	132	LYS
4	B	137	ARG
4	B	150	VAL
4	B	154	LYS
4	B	197	VAL
5	C	31	VAL
5	C	71	ASP
5	C	74	VAL
5	C	108	ILE
5	C	163	ASN
5	C	176	ASN
5	C	180	ILE
6	D	79	LEU
6	D	80	ARG
7	E	172	LYS
9	G	104	THR
9	G	154	GLU
10	H	1	MET
10	H	8	LEU
10	H	10	VAL
10	H	23	ARG
10	H	29	ILE
10	H	41	ASN
10	H	51	ILE
10	H	73	VAL
10	H	74	VAL
10	H	81	ILE
11	I	39	SER
11	I	45	LYS

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Mol	Chain	Res	Type
11	I	60	LEU
12	J	8	THR
12	J	88	LYS
13	K	3	HIS
13	K	5	LYS
13	K	28	LEU
13	K	37	THR
13	K	48	VAL
13	K	54	THR
13	K	75	VAL
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
15	M	20	HIS
15	M	25	PRO
15	M	31	ASP
15	M	54	VAL
15	M	85	SER
15	M	92	THR
15	M	99	VAL
16	N	9	VAL
16	N	15	LYS
16	N	17	VAL
16	N	22	LYS
16	N	30	LYS
16	N	93	LYS
16	N	98	ILE
17	O	5	ILE
17	O	18	ASP
17	O	87	ARG
18	P	32	ARG
18	P	65	SER
18	P	102	THR
18	P	124	ILE
18	P	125	THR

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Mol	Chain	Res	Type
18	P	126	ILE
19	Q	5	ASP
19	Q	7	LEU
19	Q	12	ILE
19	Q	29	VAL
19	Q	36	THR
20	R	10	HIS
20	R	11	ASN
20	R	55	THR
21	S	13	LYS
21	S	71	MET
22	T	15	ASP
22	T	62	LEU
23	U	32	ARG
23	U	35	THR
23	U	37	ILE
23	U	78	ILE
25	W	46	THR
26	Z	12	SER
26	Z	41	LEU
26	Z	58	LEU
27	1	8	ILE
27	1	9	ILE
27	1	15	SER
27	1	34	LYS
27	1	54	LYS
28	2	10	ARG
28	2	15	THR
28	2	42	LEU
28	2	44	VAL
29	3	31	HIS
29	3	39	ASP
29	3	46	LYS
29	3	49	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	155	GLN
3	A	167	GLN
3	A	199	ASN
4	B	35	GLN

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Mol	Chain	Res	Type
4	B	48	GLN
4	B	129	HIS
4	B	169	ASN
4	B	192	ASN
5	C	98	GLN
5	C	112	GLN
5	C	132	ASN
5	C	163	ASN
5	C	176	ASN
6	D	37	ASN
6	D	63	GLN
7	E	61	HIS
9	G	73	ASN
9	G	107	GLN
9	G	129	HIS
9	G	145	HIS
10	H	26	ASN
10	H	41	ASN
10	H	46	HIS
10	H	79	HIS
11	I	66	ASN
12	J	46	ASN
12	J	47	GLN
13	K	61	HIS
14	L	41	GLN
14	L	97	HIS
16	N	14	HIS
16	N	37	GLN
16	N	41	ASN
16	N	52	ASN
16	N	72	HIS
16	N	81	ASN
17	O	89	ASN
18	P	17	GLN
18	P	73	ASN
18	P	81	HIS
18	P	82	ASN
20	R	29	HIS
20	R	44	GLN
20	R	71	GLN
21	S	99	HIS
21	S	105	GLN

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Mol	Chain	Res	Type
21	S	121	GLN
22	T	12	ASN
22	T	35	ASN
22	T	57	HIS
22	T	71	ASN
26	Z	29	ASN
26	Z	44	HIS
28	2	29	ASN
29	3	7	HIS
29	3	33	ASN
30	4	13	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2647/2880 (91%)	474 (17%)	54 (2%)
2	Y	119/123 (96%)	18 (15%)	0
All	All	2766/3003 (92%)	492 (17%)	54 (1%)

All (492) 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

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Mol	Chain	Res	Type
1	X	100	G
1	X	101	A
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

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Mol	Chain	Res	Type
1	X	425	A
1	X	441	A
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

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Mol	Chain	Res	Type
1	X	633	G
1	X	636	G
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

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Mol	Chain	Res	Type
1	X	841	G
1	X	859	U
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

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Mol	Chain	Res	Type
1	X	1099	A
1	X	1108	U
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

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Mol	Chain	Res	Type
1	X	1359	G
1	X	1378	A
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

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Mol	Chain	Res	Type
1	X	1602	G
1	X	1608	U
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	1781	C
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

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Mol	Chain	Res	Type
1	X	1831	G
1	X	1842	G
1	X	1868	A
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

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Mol	Chain	Res	Type
1	X	2052	G
1	X	2075	U
1	X	2083	G
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

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Mol	Chain	Res	Type
1	X	2402	U
1	X	2404	A
1	X	2405	A
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

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Mol	Chain	Res	Type
1	X	2668	U
1	X	2691	C
1	X	2692	A
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

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Mol	Chain	Res	Type
2	Y	28	A
2	Y	43	G
2	Y	44	C
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

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Mol	Chain	Res	Type
1	X	1441	A
1	X	1442	C
1	X	1496	G
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 oligosaccharides 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	-	59,60,60	5.01	27 (45%)	77,90,90	1.35	6 (7%)

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	-	-	19/80/115/115	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	2881	LMA	C30-C2	-20.18	1.10	1.53
31	X	2881	LMA	C2-C1	-17.55	1.13	1.51
31	X	2881	LMA	O53-C8	-10.18	1.25	1.43
31	X	2881	LMA	O2-C13	8.68	1.57	1.44
31	X	2881	LMA	C35-C12	-8.40	1.36	1.53
31	X	2881	LMA	C33-C8	-8.16	1.41	1.52
31	X	2881	LMA	C7-C6	-7.19	1.44	1.54
31	X	2881	LMA	C19-C16	-6.53	1.38	1.52
31	X	2881	LMA	C8-C9	-5.87	1.41	1.54
31	X	2881	LMA	C32-C6	-5.80	1.38	1.53
31	X	2881	LMA	O5-C16	-5.51	1.34	1.44
31	X	2881	LMA	C16-C17	-5.25	1.41	1.53
31	X	2881	LMA	C40-C23	-4.96	1.43	1.53
31	X	2881	LMA	O55-C54	4.84	1.38	1.21
31	X	2881	LMA	C6-C5	4.58	1.61	1.53
31	X	2881	LMA	O52-C51	4.49	1.37	1.21
31	X	2881	LMA	O51-C17	-4.40	1.37	1.45
31	X	2881	LMA	O2-C1	3.84	1.43	1.34
31	X	2881	LMA	C2-C3	3.81	1.63	1.54
31	X	2881	LMA	C12-C13	-3.71	1.44	1.54
31	X	2881	LMA	O17-C24	3.31	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	2881	LMA	O3-C3	2.78	1.50	1.43
31	X	2881	LMA	O4-C18	2.24	1.49	1.44
31	X	2881	LMA	C4-C5	2.23	1.59	1.54
31	X	2881	LMA	C15-C16	2.20	1.57	1.52
31	X	2881	LMA	O12-C54	2.07	1.39	1.35
31	X	2881	LMA	O7-C5	2.03	1.49	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X	2881	LMA	O12-C54-C56	4.73	119.52	111.09
31	X	2881	LMA	O51-C51-C53	4.70	119.48	111.09
31	X	2881	LMA	O7-C5-C4	3.96	112.90	108.23
31	X	2881	LMA	C3-C2-C1	-2.75	104.38	109.93
31	X	2881	LMA	C58-C57-C36	-2.62	109.42	113.68
31	X	2881	LMA	C25-C24-C23	-2.50	106.55	112.97

There are no chirality outliers.

All (19) torsion outliers are listed below:

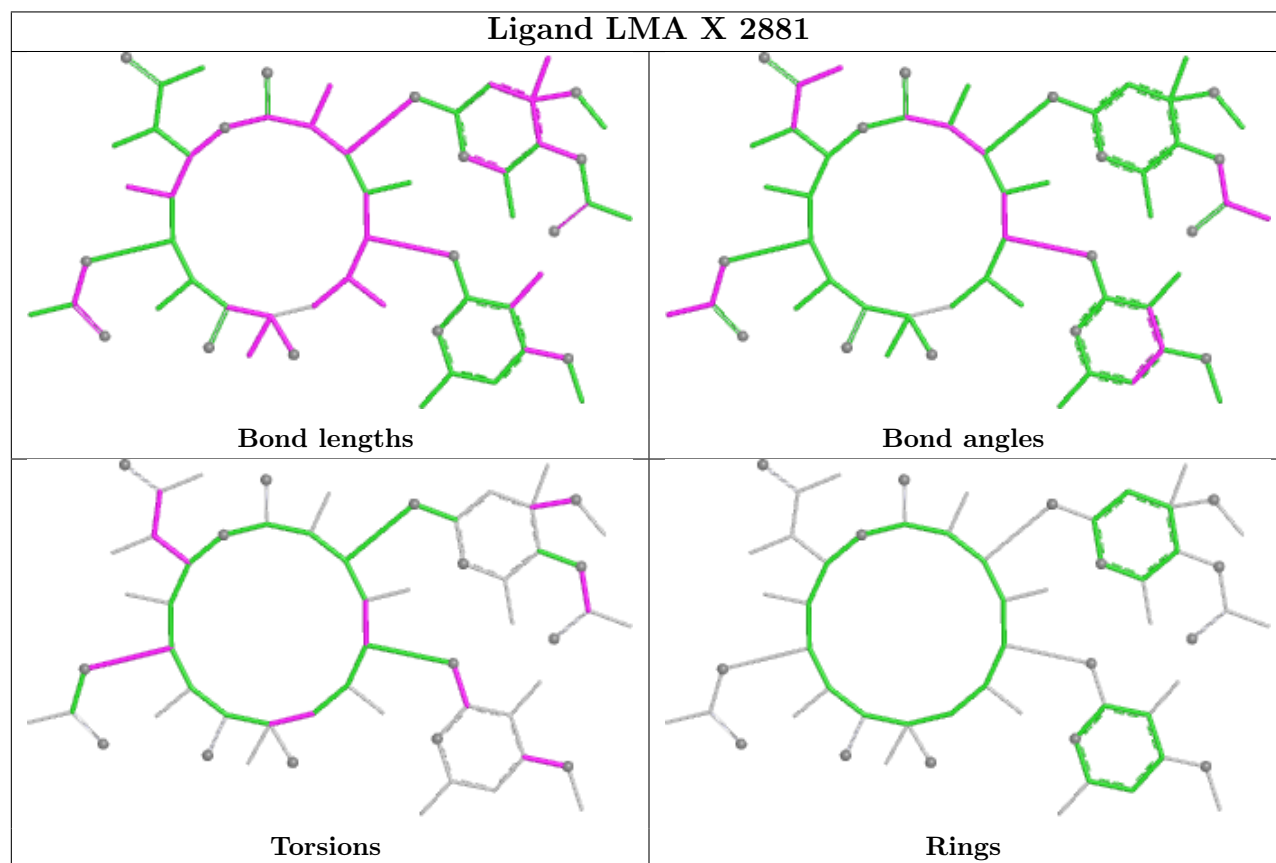
Mol	Chain	Res	Type	Atoms
31	X	2881	LMA	C3-C4-C5-C6
31	X	2881	LMA	C3-C4-C5-O7
31	X	2881	LMA	C31-C4-C5-C6
31	X	2881	LMA	C6-C7-C8-C9
31	X	2881	LMA	C12-C11-O12-C54
31	X	2881	LMA	C13-C36-C57-O57
31	X	2881	LMA	C13-C36-C57-C58
31	X	2881	LMA	C37-C36-C57-O57
31	X	2881	LMA	C37-C36-C57-C58
31	X	2881	LMA	C53-C51-O51-C17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

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	2657/2880 (92%)	0.92	458 (17%) 4 3	32, 91, 207, 392	0
2	Y	120/123 (97%)	1.35	30 (25%) 2 2	85, 155, 211, 300	0
3	A	253/274 (92%)	1.97	99 (39%) 1 1	54, 119, 183, 297	0
4	B	205/211 (97%)	0.75	23 (11%) 10 7	22, 64, 130, 298	0
5	C	194/205 (94%)	1.65	65 (33%) 1 1	44, 117, 220, 268	0
6	D	177/180 (98%)	2.11	83 (46%) 0 1	146, 209, 280, 370	0
7	E	171/185 (92%)	1.69	60 (35%) 1 1	86, 149, 209, 245	0
8	F	63/144 (43%)	3.00	43 (68%) 0 0	180, 261, 394, 440	0
9	G	142/174 (81%)	1.97	59 (41%) 0 1	55, 101, 188, 266	0
10	H	134/134 (100%)	0.32	6 (4%) 38 24	35, 61, 108, 204	0
11	I	134/156 (85%)	2.41	67 (50%) 0 1	64, 145, 237, 367	0
12	J	136/141 (96%)	1.63	43 (31%) 1 1	76, 108, 190, 272	0
13	K	113/116 (97%)	0.25	7 (6%) 26 17	27, 46, 79, 105	0
14	L	104/114 (91%)	2.13	45 (43%) 0 1	117, 160, 248, 306	0
15	M	108/166 (65%)	0.63	11 (10%) 12 8	36, 60, 135, 241	0
16	N	117/118 (99%)	1.21	22 (18%) 3 3	44, 88, 156, 279	0
17	O	94/100 (94%)	1.69	30 (31%) 1 1	58, 119, 195, 238	0
18	P	126/134 (94%)	0.38	8 (6%) 26 17	29, 59, 118, 200	0
19	Q	93/95 (97%)	1.54	33 (35%) 1 1	59, 107, 182, 273	0
20	R	110/115 (95%)	2.14	46 (41%) 0 1	68, 127, 234, 359	0
21	S	175/237 (73%)	1.93	66 (37%) 1 1	112, 169, 237, 314	0
22	T	74/91 (81%)	1.86	20 (27%) 1 1	82, 123, 199, 271	0
23	U	72/81 (88%)	2.90	43 (59%) 0 0	89, 155, 302, 332	0
24	V	65/67 (97%)	1.03	9 (13%) 6 5	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%)	1.10	11 (20%) 3 2	73, 102, 166, 177	0
26	Z	57/60 (95%)	0.92	10 (17%) 4 3	31, 63, 108, 191	0
27	1	53/55 (96%)	3.67	38 (71%) 0 0	106, 171, 261, 319	0
28	2	46/47 (97%)	1.69	16 (34%) 1 1	56, 85, 154, 195	0
29	3	59/66 (89%)	4.09	51 (86%) 0 0	97, 150, 276, 316	0
30	4	37/37 (100%)	3.70	25 (67%) 0 0	133, 223, 289, 323	0
All	All	5944/6561 (90%)	1.32	1527 (25%) 1 2	22, 105, 230, 440	0

All (1527) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	9	MET	14.3
3	A	243	ALA	12.2
3	A	161	GLY	11.6
21	S	92	VAL	11.5
29	3	44	LYS	11.3
23	U	47	HIS	10.6
1	X	2290	A	10.2
27	1	35	LEU	10.0
11	I	36	GLY	10.0
3	A	85	TYR	9.8
29	3	7	HIS	9.7
27	1	24	THR	9.7
12	J	84	MET	9.6
22	T	13	GLY	9.6
22	T	15	ASP	9.4
11	I	88	PHE	9.3
3	A	86	ASP	9.3
1	X	2190	A	9.2
27	1	13	GLU	9.1
14	L	55	SER	9.1
29	3	14	ILE	9.1
15	M	29	PRO	9.0
23	U	30	VAL	8.9
1	X	304	A	8.8
4	B	135	HIS	8.8
9	G	110	LEU	8.7
3	A	251	TRP	8.7
27	1	47	HIS	8.6
3	A	221	HIS	8.4

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Mol	Chain	Res	Type	RSRZ
8	F	126	THR	8.4
11	I	46	GLY	8.2
1	X	2044	G	8.2
17	O	36	LYS	8.1
14	L	34	SER	8.0
10	H	27	SER	8.0
12	J	27	TYR	7.9
30	4	37	GLY	7.9
11	I	54	SER	7.9
30	4	5	SER	7.8
11	I	48	PHE	7.7
9	G	109	GLY	7.7
30	4	24	LEU	7.7
3	A	204	ASN	7.6
6	D	40	LEU	7.6
27	1	36	GLU	7.6
8	F	91	PRO	7.5
22	T	18	PRO	7.5
20	R	67	GLY	7.3
23	U	60	VAL	7.3
17	O	39	PHE	7.3
30	4	16	VAL	7.3
23	U	52	ARG	7.2
1	X	1830	C	7.2
1	X	656	U	7.1
1	X	2043	A	7.1
30	4	18	ARG	7.1
3	A	242	GLY	7.1
1	X	2370	G	7.1
3	A	271	ILE	7.1
5	C	19	LEU	7.0
1	X	1055	A	7.0
7	E	5	GLY	7.0
25	W	35	SER	7.0
1	X	2731	G	6.9
1	X	1059	A	6.9
5	C	44	SER	6.9
6	D	42	SER	6.9
11	I	52	GLY	6.9
23	U	31	GLY	6.9
27	1	22	TYR	6.8
30	4	2	LYS	6.8

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Mol	Chain	Res	Type	RSRZ
20	R	94	VAL	6.8
27	1	27	ASN	6.8
5	C	48	ARG	6.7
1	X	2299	A	6.7
23	U	46	LEU	6.7
14	L	64	LYS	6.7
1	X	1082	G	6.7
21	S	32	PHE	6.7
1	X	1574	A	6.7
23	U	65	ASN	6.7
16	N	91	ASN	6.6
1	X	1080	A	6.6
1	X	1104	G	6.6
29	3	10	ALA	6.6
8	F	130	THR	6.6
7	E	37	TYR	6.5
27	1	52	GLU	6.4
1	X	69	G	6.4
12	J	85	GLY	6.4
14	L	35	SER	6.4
17	O	23	GLU	6.4
22	T	16	SER	6.4
21	S	94	VAL	6.4
9	G	97	ASP	6.4
29	3	64	ARG	6.3
1	X	1919	A	6.3
30	4	35	ARG	6.3
9	G	34	PRO	6.3
16	N	23	GLY	6.2
28	2	40	HIS	6.2
1	X	1099	A	6.2
12	J	28	VAL	6.1
22	T	19	LYS	6.1
27	1	32	GLN	6.1
20	R	83	LEU	6.1
1	X	1037	U	6.1
1	X	2286	G	6.1
27	1	45	LYS	6.1
4	B	153	GLY	6.0
8	F	114	ASP	6.0
29	3	13	ARG	6.0
30	4	36	GLN	6.0

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Mol	Chain	Res	Type	RSRZ
5	C	172	VAL	6.0
8	F	123	ALA	6.0
1	X	2015	G	6.0
20	R	63	THR	6.0
5	C	164	VAL	6.0
1	X	1083	C	6.0
8	F	133	SER	6.0
1	X	154	U	6.0
11	I	53	ARG	5.9
7	E	17	VAL	5.9
7	E	65	HIS	5.9
2	Y	68	A	5.9
12	J	136	GLU	5.9
30	4	3	VAL	5.9
7	E	143	GLN	5.9
9	G	39	GLN	5.9
11	I	74	VAL	5.8
27	1	20	PHE	5.8
27	1	2	ALA	5.8
1	X	2287	G	5.8
3	A	250	PRO	5.8
4	B	205	SER	5.8
5	C	66	ASN	5.8
29	3	6	THR	5.7
29	3	33	ASN	5.7
3	A	220	PRO	5.7
1	X	871	U	5.7
1	X	1409	U	5.7
9	G	160	ALA	5.7
30	4	23	VAL	5.7
29	3	48	PHE	5.7
1	X	983	G	5.7
15	M	28	ARG	5.7
1	X	1107	A	5.7
7	E	68	THR	5.7
9	G	53	ARG	5.7
16	N	88	ILE	5.7
1	X	248	A	5.6
23	U	79	GLU	5.6
2	Y	58	G	5.6
3	A	90	SER	5.6
26	Z	5	PRO	5.6

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Mol	Chain	Res	Type	RSRZ
17	O	5	ILE	5.6
6	D	20	PHE	5.5
29	3	54	GLU	5.5
5	C	190	ALA	5.5
11	I	32	ARG	5.5
8	F	76	TYR	5.5
5	C	47	THR	5.5
30	4	17	VAL	5.5
9	G	162	LYS	5.5
20	R	57	ASN	5.5
15	M	39	VAL	5.5
6	D	71	LYS	5.5
11	I	31	GLY	5.5
20	R	77	HIS	5.5
1	X	1068	A	5.4
20	R	113	THR	5.4
1	X	1031	C	5.4
29	3	46	LYS	5.4
21	S	77	ALA	5.4
3	A	152	LYS	5.4
1	X	101	A	5.4
21	S	1	MET	5.4
29	3	43	GLY	5.4
29	3	31	HIS	5.4
29	3	62	LEU	5.3
1	X	1095	A	5.3
11	I	57	ILE	5.3
5	C	166	TRP	5.3
3	A	88	ASN	5.3
12	J	91	VAL	5.3
14	L	52	ALA	5.3
1	X	2195	C	5.3
29	3	49	VAL	5.3
9	G	66	HIS	5.3
5	C	167	VAL	5.2
22	T	14	ARG	5.2
23	U	45	ASN	5.2
12	J	72	ASP	5.2
21	S	30	VAL	5.2
5	C	189	ASP	5.2
21	S	31	SER	5.2
1	X	1432	G	5.2

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Mol	Chain	Res	Type	RSRZ
29	3	25	PHE	5.2
8	F	127	VAL	5.2
23	U	34	THR	5.2
1	X	1120	C	5.1
3	A	34	LEU	5.1
7	E	6	LYS	5.1
16	N	92	ARG	5.1
1	X	70	A	5.1
14	L	65	THR	5.1
26	Z	38	GLY	5.1
4	B	129	HIS	5.1
21	S	127	PRO	5.1
1	X	2385	U	5.1
11	I	97	ARG	5.1
23	U	27	ASP	5.1
17	O	64	GLY	5.1
26	Z	4	HIS	5.1
23	U	78	ILE	5.0
19	Q	86	GLN	5.0
27	1	26	LYS	5.0
1	X	2189	A	5.0
11	I	56	LEU	5.0
1	X	558	G	5.0
14	L	89	PHE	5.0
6	D	125	ARG	5.0
1	X	938	G	4.9
2	Y	111	C	4.9
5	C	116	LYS	4.9
6	D	43	SER	4.9
8	F	115	LEU	4.9
1	X	1089	C	4.9
28	2	37	LYS	4.9
27	1	40	TYR	4.9
6	D	145	MET	4.9
30	4	31	LYS	4.9
21	S	125	PRO	4.9
4	B	91	VAL	4.9
29	3	45	GLY	4.8
20	R	51	VAL	4.8
20	R	58	VAL	4.8
1	X	1019	U	4.8
7	E	38	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
1	X	1105	U	4.8
6	D	120	ASN	4.8
9	G	103	TYR	4.8
27	1	21	TYR	4.8
2	Y	46	G	4.8
6	D	39	GLY	4.8
11	I	45	LYS	4.8
1	X	459	A	4.8
16	N	89	ASP	4.8
23	U	13	LEU	4.8
11	I	100	ARG	4.8
14	L	39	TYR	4.7
1	X	2079	A	4.7
3	A	32	LYS	4.7
29	3	22	VAL	4.7
8	F	125	ASN	4.7
30	4	1	MET	4.7
14	L	111	GLY	4.7
7	E	24	PHE	4.7
29	3	30	ARG	4.7
1	X	1073	G	4.7
1	X	1288	A	4.7
13	K	94	TYR	4.7
21	S	23	ALA	4.7
27	1	23	THR	4.7
3	A	92	ARG	4.7
1	X	1433	A	4.7
12	J	63	GLY	4.6
3	A	199	ASN	4.6
19	Q	64	ARG	4.6
9	G	129	HIS	4.6
11	I	21	ARG	4.6
16	N	51	ARG	4.6
29	3	50	LEU	4.6
1	X	100	G	4.6
1	X	1067	G	4.6
1	X	2194	A	4.6
8	F	113	PRO	4.6
21	S	91	PRO	4.6
6	D	121	ALA	4.6
20	R	96	LYS	4.6
1	X	434	C	4.6

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Mol	Chain	Res	Type	RSRZ
1	X	2087	U	4.5
29	3	21	LYS	4.5
20	R	52	ASN	4.5
5	C	173	ALA	4.5
8	F	111	LYS	4.5
15	M	57	ILE	4.5
1	X	1108	U	4.5
28	2	46	ASP	4.5
9	G	41	TRP	4.5
3	A	101	GLY	4.5
23	U	51	ILE	4.5
1	X	1074	G	4.5
1	X	1937	G	4.5
3	A	238	GLU	4.5
9	G	165	VAL	4.5
20	R	59	LYS	4.5
27	1	19	GLY	4.5
20	R	92	THR	4.5
5	C	59	TYR	4.5
12	J	86	LYS	4.5
17	O	14	VAL	4.5
1	X	134	G	4.5
1	X	359	G	4.5
12	J	29	ALA	4.5
1	X	1250	A	4.5
1	X	1429	A	4.5
12	J	21	ASP	4.4
23	U	16	ASN	4.4
1	X	1062	G	4.4
20	R	112	LYS	4.4
16	N	48	ARG	4.4
1	X	1084	A	4.4
1	X	1801	C	4.4
1	X	1076	U	4.4
1	X	38	G	4.4
8	F	101	TRP	4.4
28	2	42	LEU	4.4
1	X	2705	A	4.4
4	B	72	VAL	4.4
1	X	1531	C	4.4
1	X	2199	C	4.4
1	X	1077	U	4.4

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Mol	Chain	Res	Type	RSRZ
9	G	107	GLN	4.4
23	U	61	TRP	4.4
20	R	102	LYS	4.4
1	X	1602	G	4.4
14	L	87	VAL	4.4
30	4	25	VAL	4.4
17	O	11	GLN	4.4
1	X	1060	C	4.4
1	X	1593	C	4.4
29	3	55	TRP	4.4
1	X	1116	U	4.4
9	G	100	TYR	4.4
4	B	204	ALA	4.3
1	X	50	G	4.3
1	X	1098	G	4.3
5	C	42	THR	4.3
5	C	161	ALA	4.3
7	E	63	ALA	4.3
1	X	1912	G	4.3
2	Y	26	G	4.3
16	N	52	ASN	4.3
19	Q	87	SER	4.3
27	1	14	SER	4.3
11	I	121	HIS	4.3
19	Q	65	VAL	4.3
20	R	81	VAL	4.3
4	B	18	ASP	4.3
9	G	67	ARG	4.3
1	X	1792	C	4.3
21	S	126	GLY	4.3
3	A	45	ASN	4.3
22	T	12	ASN	4.3
14	L	17	VAL	4.3
1	X	1092	U	4.2
1	X	537	C	4.2
1	X	1086	C	4.2
27	1	44	ALA	4.2
30	4	26	ILE	4.2
7	E	83	TYR	4.2
6	D	179	LYS	4.2
16	N	84	LYS	4.2
15	M	40	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
5	C	121	ASP	4.2
12	J	88	LYS	4.2
3	A	272	VAL	4.2
9	G	161	GLN	4.2
20	R	69	GLN	4.2
9	G	90	LEU	4.2
4	B	202	ALA	4.2
12	J	22	ALA	4.2
14	L	58	ALA	4.2
11	I	50	GLU	4.2
20	R	66	GLN	4.2
11	I	73	GLU	4.2
1	X	1023	U	4.2
1	X	1810	U	4.2
14	L	56	SER	4.2
14	L	63	ASN	4.2
14	L	107	ALA	4.2
21	S	130	ILE	4.2
1	X	1065	A	4.2
3	A	97	HIS	4.2
29	3	63	PRO	4.2
1	X	759	C	4.2
29	3	26	LYS	4.2
1	X	1085	G	4.2
1	X	969	U	4.1
22	T	73	GLY	4.1
1	X	1100	G	4.1
1	X	2203	G	4.1
14	L	62	GLY	4.1
4	B	84	PHE	4.1
1	X	178	C	4.1
1	X	1087	C	4.1
29	3	39	ASP	4.1
30	4	6	SER	4.1
21	S	157	GLY	4.1
23	U	35	THR	4.1
5	C	57	LYS	4.1
11	I	76	LYS	4.1
18	P	19	LYS	4.1
1	X	1883	A	4.1
16	N	94	VAL	4.1
28	2	43	THR	4.1

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Mol	Chain	Res	Type	RSRZ
3	A	189	GLU	4.1
1	X	1058	G	4.1
1	X	1332	G	4.1
1	X	2447	G	4.1
29	3	42	ARG	4.1
9	G	65	LYS	4.0
23	U	39	LYS	4.0
1	X	483	A	4.0
3	A	160	ALA	4.0
21	S	21	ALA	4.0
5	C	174	GLY	4.0
11	I	22	GLY	4.0
1	X	1428	G	4.0
9	G	33	ILE	4.0
29	3	12	ARG	4.0
14	L	54	ALA	4.0
3	A	217	GLY	4.0
8	F	78	ILE	4.0
10	H	57	ASP	4.0
27	1	50	PHE	4.0
8	F	117	ALA	4.0
20	R	82	ALA	4.0
1	X	1553	G	4.0
5	C	171	PRO	4.0
15	M	34	ARG	4.0
11	I	114	ILE	4.0
29	3	16	ILE	4.0
14	L	20	THR	4.0
28	2	45	SER	4.0
6	D	57	LEU	4.0
10	H	28	GLY	4.0
1	X	1435	G	4.0
14	L	67	THR	4.0
27	1	31	THR	4.0
7	E	25	LYS	4.0
9	G	163	PRO	3.9
21	S	106	GLY	3.9
1	X	1069	G	3.9
1	X	1781	C	3.9
6	D	117	ILE	3.9
1	X	1505	U	3.9
2	Y	54	U	3.9

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Mol	Chain	Res	Type	RSRZ
17	O	10	LYS	3.9
25	W	39	ALA	3.9
19	Q	55	THR	3.9
6	D	75	SER	3.9
1	X	219	G	3.9
1	X	492	G	3.9
1	X	2867	G	3.9
30	4	20	HIS	3.9
3	A	96	LEU	3.9
1	X	1093	U	3.9
2	Y	16	U	3.9
14	L	12	ARG	3.9
8	F	94	ALA	3.9
6	D	30	ARG	3.9
1	X	1115	C	3.9
1	X	2085	G	3.9
1	X	2760	G	3.9
21	S	86	VAL	3.9
5	C	188	ILE	3.9
22	T	74	LYS	3.9
17	O	13	ARG	3.8
11	I	26	THR	3.8
12	J	82	THR	3.8
23	U	29	GLY	3.8
28	2	38	GLY	3.8
20	R	98	ILE	3.8
1	X	1495	G	3.8
1	X	1871	G	3.8
3	A	155	GLN	3.8
18	P	8	PHE	3.8
19	Q	62	ARG	3.8
21	S	76	ARG	3.8
6	D	126	GLY	3.8
11	I	33	GLY	3.8
11	I	65	PHE	3.8
1	X	1106	A	3.8
1	X	1920	A	3.8
17	O	21	ARG	3.8
7	E	58	ALA	3.8
8	F	124	ALA	3.8
1	X	398	C	3.8
1	X	411	C	3.8

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Mol	Chain	Res	Type	RSRZ
1	X	559	C	3.8
1	X	2842	C	3.8
7	E	23	VAL	3.8
6	D	41	GLY	3.8
28	2	41	GLN	3.8
1	X	1799	A	3.8
1	X	1909	U	3.8
2	Y	42	U	3.8
5	C	115	GLY	3.8
1	X	1121	G	3.8
22	T	61	ALA	3.8
11	I	115	SER	3.8
19	Q	56	MET	3.8
1	X	601	A	3.8
1	X	1921	A	3.8
9	G	91	THR	3.8
9	G	111	LYS	3.7
1	X	1613	G	3.7
11	I	90	ARG	3.7
25	W	7	ARG	3.7
7	E	41	LEU	3.7
9	G	71	THR	3.7
2	Y	110	U	3.7
23	U	57	VAL	3.7
1	X	1096	A	3.7
1	X	1603	A	3.7
6	D	66	ILE	3.7
14	L	108	ARG	3.7
29	3	37	SER	3.7
3	A	22	PHE	3.7
22	T	20	TYR	3.7
1	X	424	G	3.7
1	X	1333	G	3.7
1	X	1562	G	3.7
1	X	2846	G	3.7
1	X	177	U	3.7
1	X	2016	A	3.7
15	M	30	GLY	3.7
1	X	1606	C	3.7
23	U	8	THR	3.7
1	X	940	G	3.7
7	E	33	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
17	O	30	GLY	3.7
1	X	1812	U	3.7
8	F	88	SER	3.7
9	G	159	SER	3.7
21	S	24	TYR	3.7
28	2	5	TYR	3.7
1	X	724	C	3.7
3	A	28	LYS	3.7
26	Z	8	LYS	3.7
25	W	33	GLU	3.6
1	X	1365	U	3.6
9	G	74	MET	3.6
7	E	111	HIS	3.6
30	4	21	GLY	3.6
6	D	139	PRO	3.6
1	X	1923	U	3.6
20	R	9	HIS	3.6
3	A	244	GLY	3.6
1	X	1867	A	3.6
5	C	162	ARG	3.6
1	X	246	C	3.6
3	A	206	VAL	3.6
1	X	2291	U	3.6
1	X	1102	G	3.6
1	X	2581	A	3.6
1	X	2737	A	3.6
18	P	11	LYS	3.6
1	X	2196	U	3.6
3	A	98	TYR	3.6
27	1	41	ASP	3.6
1	X	1126	A	3.5
1	X	2289	A	3.5
1	X	2481	G	3.5
3	A	24	GLY	3.5
23	U	14	VAL	3.5
1	X	557	U	3.5
1	X	2285	U	3.5
10	H	46	HIS	3.5
17	O	78	VAL	3.5
1	X	1079	G	3.5
1	X	1193	G	3.5
1	X	358	C	3.5

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Mol	Chain	Res	Type	RSRZ
1	X	661	C	3.5
23	U	54	ASN	3.5
4	B	128	SER	3.5
21	S	105	GLN	3.5
20	R	7	GLY	3.5
29	3	8	LYS	3.5
6	D	54	ALA	3.5
5	C	185	ARG	3.5
1	X	1605	A	3.5
3	A	46	ASN	3.5
1	X	1398	G	3.5
9	G	108	GLY	3.5
14	L	30	SER	3.5
7	E	89	LEU	3.5
11	I	55	ARG	3.5
5	C	178	TYR	3.5
6	D	72	LYS	3.5
7	E	60	LYS	3.5
1	X	1032	A	3.5
1	X	2045	A	3.5
21	S	22	VAL	3.5
29	3	60	LEU	3.5
1	X	514	G	3.5
1	X	733	G	3.5
21	S	44	ARG	3.5
1	X	2080	U	3.5
3	A	69	LYS	3.4
7	E	42	THR	3.4
8	F	87	GLY	3.4
5	C	134	ILE	3.4
8	F	107	ILE	3.4
11	I	18	ARG	3.4
1	X	2204	A	3.4
2	Y	17	A	3.4
1	X	2295	C	3.4
1	X	1357	U	3.4
1	X	1886	G	3.4
1	X	2217	G	3.4
8	F	136	VAL	3.4
17	O	46	VAL	3.4
3	A	35	THR	3.4
23	U	43	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
11	I	17	LYS	3.4
7	E	133	VAL	3.4
11	I	120	VAL	3.4
5	C	17	LEU	3.4
1	X	540	G	3.4
1	X	1882	G	3.4
1	X	2363	G	3.4
7	E	64	LEU	3.4
27	1	51	ARG	3.4
17	O	37	ALA	3.4
1	X	1224	A	3.4
1	X	1954	A	3.4
2	Y	28	A	3.4
5	C	3	GLN	3.4
1	X	1103	C	3.4
2	Y	14	C	3.4
1	X	1119	U	3.4
1	X	2081	U	3.4
8	F	99	LEU	3.4
21	S	40	ASP	3.4
1	X	59	G	3.4
1	X	1850	G	3.4
3	A	219	LYS	3.4
9	G	158	HIS	3.4
19	Q	94	GLN	3.4
3	A	215	TRP	3.3
1	X	2364	C	3.3
7	E	62	ARG	3.3
3	A	268	ASP	3.3
5	C	129	LYS	3.3
9	G	105	GLY	3.3
11	I	34	HIS	3.3
11	I	13	ARG	3.3
3	A	21	ASP	3.3
6	D	153	ASP	3.3
29	3	28	GLY	3.3
1	X	1467	U	3.3
1	X	1506	C	3.3
1	X	1570	C	3.3
3	A	162	THR	3.3
11	I	16	ARG	3.3
13	K	12	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	X	1841	G	3.3
8	F	134	MET	3.3
21	S	85	MET	3.3
5	C	7	ILE	3.3
11	I	41	SER	3.3
1	X	210	A	3.3
1	X	1800	A	3.3
20	R	65	PRO	3.3
4	B	136	ARG	3.3
6	D	11	GLN	3.3
12	J	12	LYS	3.3
25	W	1	MET	3.3
6	D	74	ILE	3.3
29	3	47	GLY	3.3
14	L	93	SER	3.3
3	A	29	ARG	3.3
9	G	116	ARG	3.3
20	R	93	ARG	3.3
9	G	132	PHE	3.3
27	1	18	THR	3.3
20	R	90	LYS	3.3
1	X	205	A	3.3
1	X	665	A	3.3
1	X	1071	U	3.3
1	X	1109	A	3.3
1	X	2198	U	3.3
1	X	133	C	3.3
6	D	129	ASN	3.2
1	X	34	U	3.2
1	X	423	G	3.2
1	X	1852	G	3.2
1	X	2773	G	3.2
7	E	88	GLU	3.2
11	I	11	GLY	3.2
1	X	1945	C	3.2
6	D	169	LEU	3.2
19	Q	8	GLN	3.2
5	C	130	THR	3.2
23	U	50	ALA	3.2
12	J	68	ARG	3.2
9	G	32	TYR	3.2
23	U	49	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
3	A	254	PRO	3.2
1	X	732	G	3.2
1	X	2617	G	3.2
3	A	103	LYS	3.2
6	D	78	LYS	3.2
1	X	1056	U	3.2
3	A	47	ARG	3.2
3	A	100	ASP	3.2
8	F	131	ALA	3.2
2	Y	109	G	3.2
12	J	62	GLY	3.2
27	1	34	LYS	3.2
26	Z	51	TYR	3.2
3	A	218	ARG	3.2
8	F	112	MET	3.2
21	S	132	GLN	3.2
28	2	34	ARG	3.2
25	W	31	SER	3.2
3	A	249	THR	3.2
17	O	31	ASP	3.1
20	R	56	LYS	3.1
1	X	360	A	3.1
6	D	105	ASN	3.1
21	S	25	ASN	3.1
9	G	157	PRO	3.1
1	X	203	G	3.1
1	X	1514	C	3.1
16	N	86	ALA	3.1
5	C	122	GLY	3.1
11	I	44	GLY	3.1
1	X	302	U	3.1
19	Q	72	ARG	3.1
14	L	42	ILE	3.1
11	I	81	GLN	3.1
29	3	56	ALA	3.1
5	C	45	THR	3.1
14	L	19	THR	3.1
2	Y	43	G	3.1
3	A	252	GLY	3.1
7	E	82	GLY	3.1
5	C	71	ASP	3.1
23	U	53	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
11	I	40	ARG	3.1
5	C	20	PRO	3.1
14	L	95	LYS	3.1
29	3	32	GLN	3.1
5	C	193	LEU	3.1
1	X	1468	A	3.1
2	Y	60	A	3.1
5	C	8	GLY	3.1
23	U	28	GLY	3.1
28	2	15	THR	3.1
1	X	2735	C	3.1
14	L	28	ARG	3.1
20	R	95	ARG	3.1
21	S	108	VAL	3.1
23	U	48	LYS	3.1
25	W	38	PRO	3.1
1	X	1496	G	3.1
20	R	78	ALA	3.1
1	X	616	U	3.1
2	Y	50	U	3.1
14	L	41	GLN	3.1
7	E	22	GLY	3.1
17	O	7	THR	3.1
30	4	4	ARG	3.1
3	A	201	GLU	3.1
1	X	1081	A	3.1
1	X	1437	A	3.1
1	X	1604	A	3.1
1	X	1884	A	3.1
1	X	2381	A	3.1
1	X	2728	A	3.1
1	X	2730	A	3.1
2	Y	3	A	3.1
4	B	203	LYS	3.1
21	S	93	GLU	3.1
29	3	29	LYS	3.1
7	E	114	ILE	3.1
12	J	138	TYR	3.1
1	X	1734	C	3.0
12	J	90	ALA	3.0
21	S	29	ASN	3.0
1	X	858	G	3.0

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Mol	Chain	Res	Type	RSRZ
11	I	24	GLY	3.0
29	3	38	GLY	3.0
7	E	34	THR	3.0
1	X	1733	U	3.0
1	X	2180	U	3.0
3	A	163	SER	3.0
6	D	144	ASP	3.0
12	J	26	ASP	3.0
1	X	461	A	3.0
19	Q	9	ALA	3.0
1	X	2453	C	3.0
7	E	43	VAL	3.0
20	R	103	LYS	3.0
27	1	46	LYS	3.0
4	B	14	ILE	3.0
8	F	74	MET	3.0
27	1	12	MET	3.0
1	X	1	G	3.0
1	X	1146	G	3.0
1	X	1436	G	3.0
1	X	2782	G	3.0
7	E	67	LEU	3.0
22	T	59	LEU	3.0
8	F	108	ALA	3.0
14	L	104	ALA	3.0
3	A	269	ARG	3.0
9	G	40	ASN	3.0
13	K	93	GLY	3.0
30	4	15	LYS	3.0
1	X	1607	A	3.0
1	X	1625	A	3.0
1	X	1839	A	3.0
3	A	241	THR	3.0
11	I	86	THR	3.0
1	X	2082	C	3.0
12	J	106	GLU	3.0
29	3	23	MET	3.0
14	L	59	LEU	3.0
5	C	43	ALA	3.0
7	E	135	GLY	3.0
1	X	726	G	3.0
21	S	69	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
27	1	43	VAL	3.0
6	D	138	PHE	3.0
11	I	49	PHE	3.0
1	X	1097	A	3.0
6	D	4	LEU	3.0
21	S	131	PRO	3.0
5	C	81	GLY	3.0
21	S	56	VAL	3.0
1	X	1515	U	3.0
1	X	1601	U	3.0
1	X	2197	U	3.0
21	S	147	ILE	3.0
1	X	861	G	2.9
1	X	1955	G	2.9
1	X	2361	G	2.9
11	I	23	PRO	2.9
11	I	47	ALA	2.9
7	E	13	SER	2.9
1	X	247	A	2.9
1	X	435	A	2.9
1	X	441	A	2.9
1	X	668	A	2.9
1	X	1057	A	2.9
30	4	30	VAL	2.9
3	A	175	ILE	2.9
27	1	30	ASN	2.9
1	X	118	U	2.9
1	X	1072	U	2.9
28	2	28	ARG	2.9
6	D	56	GLU	2.9
6	D	94	GLU	2.9
1	X	1527	G	2.9
1	X	1849	G	2.9
1	X	2386	G	2.9
17	O	47	PHE	2.9
1	X	774	A	2.9
1	X	1061	A	2.9
1	X	1569	A	2.9
2	Y	47	A	2.9
1	X	1522	C	2.9
6	D	84	PRO	2.9
6	D	119	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	X	2284	U	2.9
3	A	202	HIS	2.9
9	G	102	ARG	2.9
18	P	21	ARG	2.9
4	B	94	ASP	2.9
22	T	17	ASN	2.9
1	X	1114	A	2.9
1	X	1507	A	2.9
1	X	1840	A	2.9
8	F	104	VAL	2.9
1	X	2485	U	2.9
23	U	75	TYR	2.9
5	C	165	SER	2.9
11	I	98	LEU	2.9
19	Q	54	SER	2.9
21	S	109	GLN	2.9
19	Q	92	ALA	2.9
21	S	20	ALA	2.9
6	D	118	ASN	2.9
16	N	110	VAL	2.9
5	C	133	PHE	2.9
6	D	143	TYR	2.9
19	Q	27	PHE	2.9
30	4	19	ARG	2.9
1	X	1440	G	2.9
1	X	2018	G	2.9
1	X	2324	G	2.9
3	A	65	ILE	2.9
17	O	96	LEU	2.9
20	R	23	ILE	2.9
21	S	67	LYS	2.9
13	K	3	HIS	2.8
7	E	80	SER	2.8
1	X	75	C	2.8
1	X	723	C	2.8
1	X	1528	C	2.8
1	X	2205	C	2.8
3	A	91	ALA	2.8
21	S	124	ALA	2.8
8	F	121	GLU	2.8
12	J	133	VAL	2.8
30	4	7	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
11	I	63	ARG	2.8
23	U	25	ARG	2.8
28	2	22	MET	2.8
1	X	83	A	2.8
1	X	911	A	2.8
1	X	1066	G	2.8
1	X	1117	G	2.8
1	X	1866	G	2.8
1	X	1874	G	2.8
1	X	1922	U	2.8
21	S	10	PRO	2.8
9	G	69	ASP	2.8
21	S	4	THR	2.8
1	X	2876	C	2.8
24	V	59	GLU	2.8
7	E	150	LYS	2.8
14	L	36	LYS	2.8
16	N	66	ASN	2.8
9	G	153	GLY	2.8
19	Q	12	ILE	2.8
3	A	200	ALA	2.8
11	I	12	SER	2.8
14	L	33	ARG	2.8
1	X	333	A	2.8
1	X	147	G	2.8
26	Z	37	HIS	2.8
9	G	89	ALA	2.8
9	G	164	GLN	2.8
14	L	57	ALA	2.8
12	J	17	ARG	2.8
14	L	18	ARG	2.8
3	A	23	SER	2.8
20	R	86	PRO	2.8
6	D	108	LEU	2.8
8	F	77	LEU	2.8
3	A	237	GLY	2.8
6	D	173	MET	2.8
1	X	2298	U	2.8
1	X	1375	C	2.8
3	A	222	GLN	2.8
6	D	3	GLN	2.8
6	D	88	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
7	E	139	GLN	2.8
14	L	86	GLN	2.8
17	O	6	GLN	2.8
1	X	484	G	2.8
1	X	789	G	2.8
6	D	65	PRO	2.8
21	S	123	VAL	2.8
21	S	3	LEU	2.8
22	T	37	LEU	2.8
3	A	182	GLU	2.8
3	A	255	THR	2.8
6	D	122	PHE	2.7
20	R	62	MET	2.7
5	C	39	ARG	2.7
5	C	49	ALA	2.7
5	C	128	ALA	2.7
20	R	30	LYS	2.7
1	X	984	A	2.7
1	X	1856	U	2.7
1	X	1873	A	2.7
1	X	1946	U	2.7
11	I	68	VAL	2.7
5	C	125	ILE	2.7
8	F	90	THR	2.7
9	G	113	GLU	2.7
29	3	27	SER	2.7
1	X	2781	G	2.7
3	A	172	ASP	2.7
5	C	131	LYS	2.7
6	D	52	LYS	2.7
27	1	3	LYS	2.7
6	D	168	ALA	2.7
1	X	1547	U	2.7
19	Q	6	ILE	2.7
3	A	64	ARG	2.7
14	L	99	ARG	2.7
29	3	15	LYS	2.7
1	X	1501	C	2.7
4	B	73	ALA	2.7
8	F	122	ALA	2.7
21	S	14	LEU	2.7
1	X	1554	G	2.7

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Mol	Chain	Res	Type	RSRZ
1	X	1832	G	2.7
1	X	2282	G	2.7
1	X	2283	G	2.7
1	X	2316	G	2.7
20	R	60	PRO	2.7
7	E	108	GLY	2.7
12	J	109	GLY	2.7
6	D	142	THR	2.7
15	M	6	LYS	2.7
17	O	55	THR	2.7
24	V	44	ARG	2.7
29	3	34	THR	2.7
6	D	23	SER	2.7
17	O	15	SER	2.7
1	X	1112	U	2.7
1	X	2171	U	2.7
1	X	343	A	2.7
1	X	2312	A	2.7
6	D	8	TYR	2.7
8	F	128	ALA	2.7
19	Q	82	LEU	2.7
25	W	6	VAL	2.7
1	X	1552	C	2.7
1	X	1885	C	2.7
1	X	2403	C	2.7
9	G	68	PRO	2.7
20	R	71	GLN	2.7
29	3	61	MET	2.7
12	J	57	ARG	2.7
16	N	20	ARG	2.7
20	R	21	THR	2.7
1	X	1573	G	2.7
5	C	6	VAL	2.7
27	1	48	VAL	2.7
8	F	100	ASN	2.7
1	X	242	A	2.6
1	X	1556	A	2.6
15	M	44	ARG	2.6
26	Z	3	LYS	2.6
3	A	48	GLY	2.6
1	X	1052	C	2.6
1	X	1631	C	2.6

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Mol	Chain	Res	Type	RSRZ
9	G	31	THR	2.6
27	1	25	THR	2.6
22	T	33	ALA	2.6
23	U	26	ALA	2.6
7	E	61	HIS	2.6
1	X	388	G	2.6
1	X	438	G	2.6
1	X	1110	G	2.6
6	D	50	ILE	2.6
17	O	95	ILE	2.6
11	I	35	LYS	2.6
20	R	64	ASN	2.6
21	S	128	ARG	2.6
1	X	132	U	2.6
23	U	10	LYS	2.6
29	3	52	LYS	2.6
6	D	151	GLY	2.6
1	X	91	A	2.6
1	X	341	A	2.6
1	X	1378	A	2.6
1	X	2169	A	2.6
19	Q	4	TYR	2.6
11	I	61	PRO	2.6
24	V	14	PHE	2.6
7	E	59	GLN	2.6
20	R	31	GLY	2.6
19	Q	21	GLU	2.6
1	X	238	G	2.6
11	I	119	THR	2.6
18	P	15	LYS	2.6
24	V	47	ARG	2.6
3	A	188	SER	2.6
3	A	191	TYR	2.6
1	X	81	C	2.6
1	X	427	C	2.6
1	X	1113	C	2.6
11	I	84	GLU	2.6
9	G	152	ALA	2.6
1	X	1482	U	2.6
1	X	225	G	2.6
1	X	1831	G	2.6
1	X	1847	G	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	30	PRO	2.6
1	X	124	A	2.6
1	X	1953	A	2.6
1	X	2247	A	2.6
2	Y	36	A	2.6
3	A	153	GLY	2.6
12	J	16	GLY	2.6
6	D	76	ASN	2.6
19	Q	57	ASN	2.6
6	D	85	VAL	2.6
14	L	8	ARG	2.6
16	N	117	ARG	2.6
1	X	207	U	2.5
1	X	1594	U	2.5
22	T	34	GLY	2.5
23	U	55	GLY	2.5
11	I	60	LEU	2.5
20	R	74	LEU	2.5
1	X	516	G	2.5
3	A	135	ARG	2.5
6	D	5	LYS	2.5
6	D	150	ARG	2.5
16	N	85	ARG	2.5
21	S	116	VAL	2.5
21	S	137	ASP	2.5
1	X	200	A	2.5
5	C	2	ALA	2.5
1	X	1075	C	2.5
1	X	1094	C	2.5
7	E	12	PRO	2.5
1	X	447	U	2.5
1	X	2086	U	2.5
6	D	130	LEU	2.5
8	F	89	SER	2.5
11	I	79	GLN	2.5
7	E	175	LYS	2.5
14	L	16	LYS	2.5
18	P	105	ARG	2.5
27	1	38	LYS	2.5
11	I	122	VAL	2.5
6	D	51	ASP	2.5
7	E	81	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
14	L	90	ASP	2.5
30	4	12	ASP	2.5
6	D	77	PHE	2.5
1	X	1512	A	2.5
1	X	2181	A	2.5
1	X	1133	G	2.5
9	G	156	HIS	2.5
1	X	1064	C	2.5
6	D	13	ARG	2.5
6	D	148	LYS	2.5
9	G	98	LYS	2.5
11	I	64	GLY	2.5
19	Q	15	LYS	2.5
19	Q	66	GLY	2.5
19	Q	85	GLY	2.5
21	S	8	ARG	2.5
23	U	40	ARG	2.5
23	U	73	GLY	2.5
24	V	2	LYS	2.5
29	3	36	LYS	2.5
22	T	67	VAL	2.5
1	X	390	U	2.5
1	X	1182	U	2.5
1	X	1424	U	2.5
1	X	2402	U	2.5
20	R	85	ASP	2.5
29	3	58	MET	2.5
6	D	161	LYS	2.5
9	G	167	LYS	2.5
21	S	80	HIS	2.5
2	Y	41	A	2.5
4	B	142	GLY	2.5
7	E	92	VAL	2.5
1	X	1503	G	2.5
1	X	1735	G	2.5
1	X	725	C	2.5
2	Y	8	C	2.5
8	F	102	ASP	2.5
1	X	1038	U	2.5
1	X	1469	U	2.5
3	A	132	LEU	2.5
3	A	264	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
5	C	38	ARG	2.5
4	B	138	PRO	2.5
23	U	62	LEU	2.5
5	C	91	TYR	2.5
19	Q	3	HIS	2.5
6	D	93	GLY	2.5
21	S	19	ILE	2.4
1	X	493	A	2.4
3	A	31	GLU	2.4
12	J	38	MET	2.4
21	S	36	ARG	2.4
1	X	939	C	2.4
1	X	1223	G	2.4
1	X	1345	G	2.4
1	X	1502	G	2.4
1	X	1790	G	2.4
1	X	2582	G	2.4
1	X	2769	C	2.4
12	J	79	PRO	2.4
1	X	1863	U	2.4
20	R	29	HIS	2.4
5	C	175	VAL	2.4
14	L	100	VAL	2.4
17	O	9	GLY	2.4
11	I	144	GLU	2.4
19	Q	14	GLU	2.4
3	A	245	ARG	2.4
12	J	73	LYS	2.4
26	Z	9	LYS	2.4
1	X	626	A	2.4
6	D	89	VAL	2.4
11	I	42	GLY	2.4
1	X	417	C	2.4
1	X	355	G	2.4
1	X	2330	G	2.4
20	R	44	GLN	2.4
12	J	44	LYS	2.4
16	N	58	ARG	2.4
6	D	175	LEU	2.4
9	G	119	LEU	2.4
6	D	90	THR	2.4
9	G	106	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
29	3	35	GLY	2.4
5	C	67	ALA	2.4
1	X	425	A	2.4
5	C	180	ILE	2.4
6	D	49	ALA	2.4
3	A	256	LYS	2.4
9	G	93	LYS	2.4
11	I	38	LYS	2.4
5	C	123	PHE	2.4
1	X	1452	U	2.4
2	Y	4	C	2.4
6	D	62	LEU	2.4
30	4	28	SER	2.4
1	X	361	G	2.4
1	X	1125	G	2.4
1	X	1191	G	2.4
2	Y	25	G	2.4
7	E	128	PRO	2.4
23	U	59	THR	2.4
5	C	132	ASN	2.4
11	I	51	GLY	2.4
24	V	63	LYS	2.4
16	N	13	ARG	2.4
6	D	99	PHE	2.4
1	X	63	A	2.4
1	X	624	A	2.4
1	X	2405	A	2.4
13	K	114	GLU	2.4
8	F	75	SER	2.4
1	X	780	U	2.4
1	X	1732	U	2.4
7	E	162	VAL	2.4
27	1	42	PRO	2.4
1	X	1111	C	2.3
1	X	2329	C	2.3
2	Y	67	C	2.3
9	G	155	THR	2.3
17	O	8	GLY	2.3
3	A	49	ARG	2.3
19	Q	90	ALA	2.3
1	X	781	G	2.3
1	X	1184	G	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	2304	G	2.3
7	E	52	VAL	2.3
8	F	120	VAL	2.3
3	A	266	THR	2.3
6	D	44	LYS	2.3
6	D	149	THR	2.3
12	J	20	GLY	2.3
22	T	28	GLY	2.3
23	U	9	GLY	2.3
12	J	108	ALA	2.3
2	Y	30	C	2.3
14	L	66	ASP	2.3
12	J	10	PHE	2.3
14	L	51	LEU	2.3
7	E	7	GLN	2.3
19	Q	71	GLN	2.3
25	W	54	GLN	2.3
26	Z	56	GLN	2.3
9	G	154	GLU	2.3
1	X	191	G	2.3
1	X	662	G	2.3
1	X	1857	G	2.3
1	X	1951	G	2.3
1	X	2727	G	2.3
12	J	137	VAL	2.3
20	R	99	VAL	2.3
3	A	253	LYS	2.3
3	A	185	ARG	2.3
12	J	83	ARG	2.3
15	M	46	ARG	2.3
7	E	14	GLY	2.3
11	I	39	SER	2.3
19	Q	2	SER	2.3
3	A	62	LEU	2.3
9	G	36	ASN	2.3
13	K	10	LEU	2.3
21	S	119	ASN	2.3
1	X	5	A	2.3
1	X	321	A	2.3
1	X	356	A	2.3
1	X	2401	A	2.3
6	D	163	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
6	D	81	GLN	2.3
1	X	1150	C	2.3
1	X	1487	C	2.3
6	D	28	VAL	2.3
3	A	44	ARG	2.3
3	A	158	ARG	2.3
4	B	83	GLY	2.3
17	O	52	GLY	2.3
21	S	9	THR	2.3
16	N	95	LEU	2.3
1	X	107	G	2.3
1	X	151	G	2.3
1	X	152	G	2.3
1	X	2868	G	2.3
12	J	105	PHE	2.3
6	D	147	ASP	2.3
9	G	78	ASP	2.3
21	S	13	LYS	2.3
1	X	190	A	2.3
1	X	655	A	2.3
1	X	1802	A	2.3
6	D	156	ILE	2.3
27	1	6	PRO	2.3
29	3	24	ALA	2.3
1	X	418	C	2.3
9	G	54	LEU	2.3
11	I	92	THR	2.3
7	E	138	LYS	2.3
24	V	48	ARG	2.3
7	E	125	VAL	2.3
20	R	100	ASP	2.3
21	S	168	VAL	2.3
17	O	28	GLU	2.2
1	X	2214	G	2.2
1	X	2346	G	2.2
1	X	2407	G	2.2
11	I	30	ALA	2.2
1	X	1555	A	2.2
1	X	1868	A	2.2
1	X	1952	A	2.2
2	Y	27	A	2.2
2	Y	59	A	2.2

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Mol	Chain	Res	Type	RSRZ
20	R	40	LEU	2.2
5	C	157	THR	2.2
12	J	14	PHE	2.2
21	S	140	LYS	2.2
5	C	50	GLN	2.2
5	C	78	VAL	2.2
5	C	187	VAL	2.2
3	A	102	GLU	2.2
5	C	124	ASP	2.2
5	C	194	GLU	2.2
3	A	133	PRO	2.2
19	Q	91	LEU	2.2
1	X	119	G	2.2
1	X	224	G	2.2
1	X	1430	G	2.2
1	X	2832	G	2.2
2	Y	56	G	2.2
3	A	27	LYS	2.2
5	C	62	LYS	2.2
1	X	416	U	2.2
1	X	890	U	2.2
12	J	11	ARG	2.2
21	S	84	TYR	2.2
1	X	1910	A	2.2
1	X	2191	A	2.2
1	X	1132	C	2.2
5	C	150	LEU	2.2
5	C	87	LYS	2.2
12	J	78	LYS	2.2
3	A	262	ARG	2.2
28	2	19	ARG	2.2
3	A	273	THR	2.2
8	F	110	THR	2.2
7	E	110	SER	2.2
17	O	24	SER	2.2
1	X	1600	U	2.2
7	E	136	ILE	2.2
1	X	111	G	2.2
1	X	442	A	2.2
1	X	1504	G	2.2
1	X	1913	G	2.2
3	A	36	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
8	F	92	ASN	2.2
21	S	165	GLU	2.2
14	L	53	ALA	2.2
21	S	33	ALA	2.2
21	S	71	MET	2.2
3	A	184	ARG	2.2
1	X	332	C	2.2
1	X	432	C	2.2
1	X	2170	C	2.2
1	X	2305	C	2.2
2	Y	49	C	2.2
9	G	104	THR	2.2
21	S	55	THR	2.2
17	O	98	ILE	2.2
27	1	8	ILE	2.2
7	E	140	LEU	2.2
17	O	25	LEU	2.2
24	V	28	LEU	2.2
7	E	167	GLU	2.2
8	F	85	GLY	2.2
11	I	102	LYS	2.2
11	I	103	ASN	2.2
16	N	116	ALA	2.2
25	W	55	GLU	2.2
12	J	123	GLY	2.2
18	P	12	LYS	2.2
27	1	54	LYS	2.2
29	3	59	LYS	2.2
1	X	666	U	2.2
1	X	2456	U	2.2
13	K	59	ASP	2.2
19	Q	5	ASP	2.2
1	X	654	A	2.2
1	X	1753	A	2.2
1	X	2738	A	2.2
1	X	88	G	2.2
1	X	90	G	2.2
1	X	231	G	2.2
1	X	433	G	2.2
1	X	2084	G	2.2
4	B	66	HIS	2.2
3	A	149	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
21	S	135	VAL	2.1
1	X	303	C	2.1
1	X	519	C	2.1
1	X	1550	C	2.1
6	D	87	ILE	2.1
7	E	131	ILE	2.1
6	D	19	GLN	2.1
21	S	154	LEU	2.1
6	D	55	LYS	2.1
6	D	152	MET	2.1
23	U	33	LYS	2.1
11	I	112	GLY	2.1
21	S	110	GLY	2.1
23	U	21	ARG	2.1
25	W	15	ASN	2.1
1	X	1124	U	2.1
1	X	153	A	2.1
1	X	2713	A	2.1
3	A	209	LYS	2.1
1	X	105	G	2.1
1	X	399	G	2.1
1	X	1864	G	2.1
1	X	2567	G	2.1
16	N	104	GLU	2.1
12	J	30	PHE	2.1
1	X	396	U	2.1
1	X	943	U	2.1
5	C	54	THR	2.1
17	O	67	LYS	2.1
21	S	166	LEU	2.1
7	E	90	ARG	2.1
10	H	23	ARG	2.1
8	F	103	GLN	2.1
1	X	6	A	2.1
1	X	2780	A	2.1
22	T	75	GLY	2.1
29	3	20	GLY	2.1
21	S	104	SER	2.1
9	G	73	ASN	2.1
1	X	1508	G	2.1
1	X	2640	G	2.1
11	I	107	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
6	D	103	LEU	2.1
12	J	32	ASP	2.1
4	B	19	ARG	2.1
4	B	146	THR	2.1
4	B	201	ALA	2.1
18	P	17	GLN	2.1
3	A	181	GLY	2.1
9	G	64	GLY	2.1
9	G	117	GLU	2.1
3	A	267	SER	2.1
22	T	38	VAL	2.1
1	X	518	A	2.1
1	X	538	A	2.1
3	A	89	ARG	2.1
10	H	121	ARG	2.1
16	N	65	ILE	2.1
20	R	14	LEU	2.1
15	M	31	ASP	2.1
21	S	53	ASP	2.1
1	X	391	C	2.1
1	X	1844	C	2.1
1	X	2771	C	2.1
1	X	1035	G	2.1
1	X	2328	G	2.1
29	3	51	ALA	2.1
9	G	72	PRO	2.1
1	X	1034	U	2.0
23	U	11	LYS	2.0
27	1	11	LYS	2.0
14	L	61	SER	2.0
3	A	106	ILE	2.0
28	2	39	ARG	2.0
1	X	1088	A	2.0
1	X	1595	A	2.0
1	X	2246	A	2.0
1	X	2390	A	2.0
3	A	99	ALA	2.0
6	D	6	THR	2.0
6	D	27	ALA	2.0
14	L	21	THR	2.0
26	Z	53	ASP	2.0
3	A	87	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	X	126	C	2.0
1	X	148	C	2.0
1	X	1090	C	2.0
1	X	1477	C	2.0
12	J	125	LYS	2.0
7	E	26	VAL	2.0
1	X	955	G	2.0
1	X	1494	G	2.0
1	X	2083	G	2.0
7	E	69	ARG	2.0
28	2	10	ARG	2.0
19	Q	88	ILE	2.0
1	X	3	U	2.0
2	Y	57	U	2.0
8	F	116	ASN	2.0
6	D	15	ALA	2.0
7	E	39	THR	2.0
7	E	96	ALA	2.0
23	U	64	ALA	2.0
6	D	113	ASP	2.0
21	S	114	ASP	2.0
24	V	19	ASP	2.0
19	Q	32	LYS	2.0
1	X	632	A	2.0
1	X	992	A	2.0
1	X	1793	A	2.0
19	Q	37	GLU	2.0
7	E	149	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	K	X	3074	1/1	0.36	0.78	171,171,171,171	0
34	K	X	3076	1/1	0.43	0.30	100,100,100,100	0
33	NA	A	277	1/1	0.65	0.36	72,72,72,72	0
33	NA	X	3037	1/1	0.66	0.24	53,53,53,53	0
33	NA	X	3055	1/1	0.71	0.73	70,70,70,70	0
32	MG	X	2988	1/1	0.73	0.43	63,63,63,63	0
33	NA	Y	126	1/1	0.74	0.50	85,85,85,85	0
33	NA	X	3050	1/1	0.76	0.24	40,40,40,40	0
32	MG	X	3000	1/1	0.76	0.26	65,65,65,65	0
32	MG	X	2891	1/1	0.76	0.20	56,56,56,56	0
32	MG	X	2975	1/1	0.77	0.20	73,73,73,73	0
33	NA	X	3046	1/1	0.77	0.51	80,80,80,80	0
33	NA	X	3048	1/1	0.77	0.44	71,71,71,71	0
32	MG	X	3010	1/1	0.78	0.28	73,73,73,73	0
32	MG	X	2925	1/1	0.80	0.27	72,72,72,72	0
33	NA	X	3042	1/1	0.81	0.34	45,45,45,45	0
33	NA	X	3036	1/1	0.81	0.37	79,79,79,79	0
32	MG	X	3018	1/1	0.81	0.23	59,59,59,59	0
33	NA	Z	61	1/1	0.82	0.24	48,48,48,48	0
33	NA	X	3053	1/1	0.82	0.54	62,62,62,62	0
32	MG	X	2944	1/1	0.82	0.32	59,59,59,59	0
34	K	X	3077	1/1	0.82	0.24	80,80,80,80	0
33	NA	X	3038	1/1	0.83	0.36	59,59,59,59	0
33	NA	X	3067	1/1	0.83	0.14	47,47,47,47	0
32	MG	X	2956	1/1	0.84	0.32	71,71,71,71	0
33	NA	X	3057	1/1	0.84	0.93	75,75,75,75	0
32	MG	X	2904	1/1	0.84	0.39	39,39,39,39	0
34	K	X	3078	1/1	0.84	0.37	91,91,91,91	0
32	MG	X	2979	1/1	0.85	0.50	50,50,50,50	0
33	NA	X	3049	1/1	0.85	0.62	68,68,68,68	0
32	MG	X	2992	1/1	0.85	0.14	44,44,44,44	0
33	NA	X	3064	1/1	0.85	0.34	58,58,58,58	0
32	MG	X	2913	1/1	0.86	0.29	56,56,56,56	0
32	MG	X	2931	1/1	0.86	0.25	48,48,48,48	0
32	MG	X	2963	1/1	0.86	0.26	69,69,69,69	0
34	K	X	3082	1/1	0.86	0.23	98,98,98,98	0
32	MG	X	2943	1/1	0.87	0.47	29,29,29,29	0
33	NA	X	3039	1/1	0.87	0.28	51,51,51,51	0
33	NA	X	3035	1/1	0.87	0.50	50,50,50,50	0
32	MG	X	2957	1/1	0.87	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	X	2914	1/1	0.87	0.31	60,60,60,60	0
32	MG	X	2964	1/1	0.88	0.28	50,50,50,50	0
32	MG	X	2939	1/1	0.88	0.47	79,79,79,79	0
32	MG	X	3029	1/1	0.88	0.24	63,63,63,63	0
32	MG	X	3004	1/1	0.88	0.49	71,71,71,71	0
33	NA	X	3060	1/1	0.88	0.57	73,73,73,73	0
32	MG	X	2911	1/1	0.89	0.41	83,83,83,83	0
33	NA	X	3061	1/1	0.89	0.31	62,62,62,62	0
32	MG	X	2934	1/1	0.89	0.26	62,62,62,62	0
31	LMA	X	2881	58/58	0.89	0.17	22,83,114,128	0
32	MG	X	3017	1/1	0.89	0.41	70,70,70,70	0
32	MG	X	2972	1/1	0.89	0.26	65,65,65,65	0
32	MG	X	2942	1/1	0.89	0.16	74,74,74,74	0
32	MG	X	3032	1/1	0.89	0.29	74,74,74,74	0
32	MG	X	2903	1/1	0.89	0.35	51,51,51,51	0
32	MG	X	2887	1/1	0.89	0.18	37,37,37,37	0
32	MG	X	2928	1/1	0.89	0.24	41,41,41,41	0
33	NA	X	3058	1/1	0.89	0.41	69,69,69,69	0
32	MG	X	2983	1/1	0.90	0.13	23,23,23,23	0
32	MG	X	3030	1/1	0.90	0.14	66,66,66,66	0
33	NA	X	3040	1/1	0.90	0.53	70,70,70,70	0
32	MG	X	2927	1/1	0.90	0.26	55,55,55,55	0
32	MG	X	2884	1/1	0.90	0.36	38,38,38,38	0
33	NA	X	3047	1/1	0.90	0.50	75,75,75,75	0
32	MG	X	2968	1/1	0.90	0.14	56,56,56,56	0
32	MG	X	3024	1/1	0.90	0.36	68,68,68,68	0
34	K	X	3079	1/1	0.90	0.23	97,97,97,97	0
33	NA	X	3065	1/1	0.90	0.40	58,58,58,58	0
32	MG	X	2902	1/1	0.91	0.26	39,39,39,39	0
33	NA	X	3052	1/1	0.91	0.14	43,43,43,43	0
32	MG	X	3019	1/1	0.91	0.28	74,74,74,74	0
32	MG	X	3023	1/1	0.91	0.20	73,73,73,73	0
33	NA	X	3056	1/1	0.91	0.89	76,76,76,76	0
32	MG	X	2910	1/1	0.91	0.21	47,47,47,47	0
32	MG	X	2947	1/1	0.91	0.35	47,47,47,47	0
32	MG	X	2952	1/1	0.91	0.33	57,57,57,57	0
32	MG	X	2984	1/1	0.91	0.22	62,62,62,62	0
33	NA	X	3063	1/1	0.91	0.28	50,50,50,50	0
33	NA	X	3033	1/1	0.91	0.37	38,38,38,38	0
32	MG	X	2987	1/1	0.91	0.21	38,38,38,38	0
32	MG	X	2954	1/1	0.91	0.19	31,31,31,31	0
32	MG	X	2915	1/1	0.91	0.28	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	X	2997	1/1	0.91	0.13	50,50,50,50	0
33	NA	K	117	1/1	0.91	0.16	28,28,28,28	0
32	MG	X	2916	1/1	0.91	0.21	51,51,51,51	0
32	MG	X	3001	1/1	0.91	0.26	84,84,84,84	0
32	MG	X	3003	1/1	0.91	0.20	55,55,55,55	0
32	MG	X	2918	1/1	0.91	0.18	60,60,60,60	0
32	MG	X	2941	1/1	0.91	0.36	46,46,46,46	0
32	MG	X	3014	1/1	0.91	0.28	54,54,54,54	0
32	MG	X	2901	1/1	0.91	0.35	30,30,30,30	0
32	MG	X	2882	1/1	0.92	0.17	5,5,5,5	0
32	MG	X	2919	1/1	0.92	0.43	61,61,61,61	0
32	MG	X	2921	1/1	0.92	0.16	52,52,52,52	0
33	NA	X	3066	1/1	0.92	0.27	48,48,48,48	0
32	MG	X	2923	1/1	0.92	0.44	66,66,66,66	0
32	MG	X	3007	1/1	0.92	0.21	37,37,37,37	0
33	NA	X	3034	1/1	0.92	0.35	50,50,50,50	0
32	MG	X	2985	1/1	0.92	0.24	50,50,50,50	0
33	NA	X	3054	1/1	0.92	0.38	49,49,49,49	0
34	K	X	3072	1/1	0.92	0.21	104,104,104,104	0
32	MG	X	2945	1/1	0.92	0.22	32,32,32,32	0
32	MG	X	3016	1/1	0.92	0.21	39,39,39,39	0
32	MG	X	2966	1/1	0.92	0.32	60,60,60,60	0
32	MG	X	2935	1/1	0.92	0.20	55,55,55,55	0
32	MG	X	2995	1/1	0.92	0.36	42,42,42,42	0
34	K	X	3080	1/1	0.92	0.25	94,94,94,94	0
34	K	X	3081	1/1	0.92	0.25	91,91,91,91	0
32	MG	X	2900	1/1	0.92	0.16	37,37,37,37	0
32	MG	X	2981	1/1	0.93	0.36	65,65,65,65	0
32	MG	X	2898	1/1	0.93	0.19	8,8,8,8	0
32	MG	X	3031	1/1	0.93	0.16	48,48,48,48	0
33	NA	X	3069	1/1	0.93	0.46	74,74,74,74	0
32	MG	X	2908	1/1	0.93	0.23	55,55,55,55	0
32	MG	I	157	1/1	0.93	0.15	50,50,50,50	0
32	MG	X	2920	1/1	0.93	0.20	31,31,31,31	0
32	MG	X	2967	1/1	0.93	0.21	50,50,50,50	0
32	MG	X	2899	1/1	0.93	0.27	57,57,57,57	0
32	MG	X	2971	1/1	0.93	0.23	44,44,44,44	0
34	K	X	3075	1/1	0.93	0.26	68,68,68,68	0
32	MG	X	2932	1/1	0.93	0.19	31,31,31,31	0
32	MG	X	2974	1/1	0.93	0.27	37,37,37,37	0
32	MG	X	2892	1/1	0.93	0.27	30,30,30,30	0
32	MG	X	2961	1/1	0.93	0.17	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	NA	X	3041	1/1	0.93	0.33	37,37,37,37	0
32	MG	X	3026	1/1	0.93	0.21	37,37,37,37	0
33	NA	X	3043	1/1	0.93	0.23	48,48,48,48	0
34	K	X	3083	1/1	0.93	0.36	103,103,103,103	0
32	MG	X	2993	1/1	0.94	0.27	51,51,51,51	0
33	NA	Y	125	1/1	0.94	0.45	62,62,62,62	0
32	MG	X	2897	1/1	0.94	0.27	37,37,37,37	0
32	MG	X	2982	1/1	0.94	0.16	51,51,51,51	0
32	MG	X	3020	1/1	0.94	0.28	42,42,42,42	0
32	MG	X	2937	1/1	0.94	0.10	46,46,46,46	0
32	MG	X	2883	1/1	0.94	0.15	34,34,34,34	0
32	MG	X	2948	1/1	0.94	0.27	40,40,40,40	0
33	NA	X	3059	1/1	0.94	0.18	66,66,66,66	0
32	MG	X	2986	1/1	0.94	0.18	54,54,54,54	0
32	MG	X	3005	1/1	0.94	0.28	58,58,58,58	0
33	NA	X	3062	1/1	0.94	0.13	47,47,47,47	0
32	MG	X	2977	1/1	0.94	0.30	51,51,51,51	0
32	MG	X	2978	1/1	0.94	0.17	48,48,48,48	0
32	MG	X	3011	1/1	0.94	0.38	45,45,45,45	0
32	MG	X	2989	1/1	0.94	0.22	83,83,83,83	0
32	MG	X	2951	1/1	0.94	0.26	28,28,28,28	0
32	MG	X	2885	1/1	0.95	0.22	21,21,21,21	0
32	MG	X	2917	1/1	0.95	0.13	52,52,52,52	0
34	K	X	3073	1/1	0.95	0.28	57,57,57,57	0
32	MG	X	3028	1/1	0.95	0.15	65,65,65,65	0
32	MG	X	2895	1/1	0.95	0.31	19,19,19,19	0
32	MG	X	2933	1/1	0.95	0.39	59,59,59,59	0
32	MG	X	2940	1/1	0.95	0.19	34,34,34,34	0
32	MG	X	2999	1/1	0.95	0.20	49,49,49,49	0
32	MG	Y	124	1/1	0.95	0.05	40,40,40,40	0
32	MG	X	3021	1/1	0.95	0.24	70,70,70,70	0
33	NA	X	3044	1/1	0.95	0.21	48,48,48,48	0
32	MG	X	3022	1/1	0.95	0.11	43,43,43,43	0
32	MG	X	2965	1/1	0.95	0.22	42,42,42,42	0
32	MG	X	2924	1/1	0.96	0.21	26,26,26,26	0
32	MG	X	2955	1/1	0.96	0.19	54,54,54,54	0
32	MG	X	2906	1/1	0.96	0.30	43,43,43,43	0
32	MG	X	2973	1/1	0.96	0.19	30,30,30,30	0
32	MG	X	2907	1/1	0.96	0.36	66,66,66,66	0
34	K	X	3070	1/1	0.96	0.36	72,72,72,72	0
32	MG	X	2896	1/1	0.96	0.26	28,28,28,28	0
32	MG	X	2976	1/1	0.96	0.18	32,32,32,32	0

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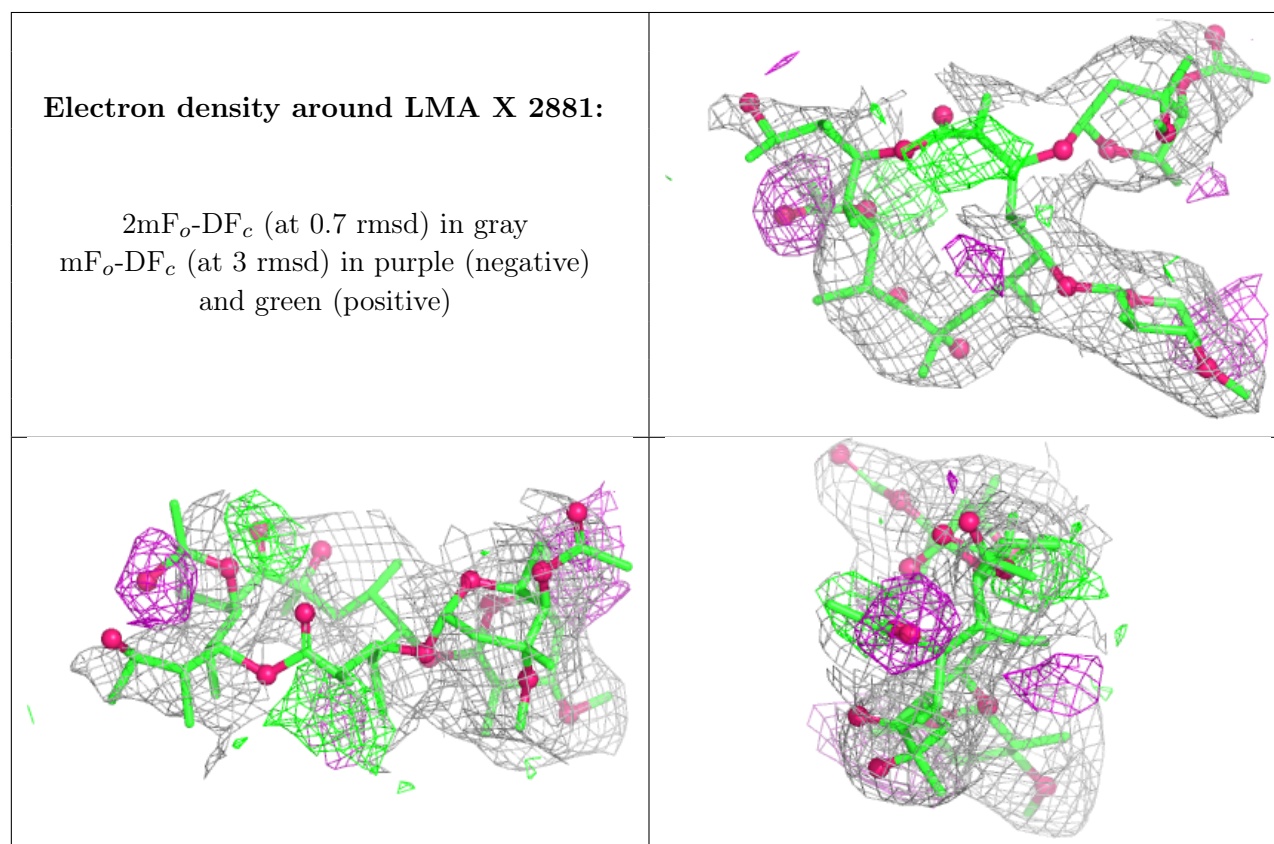
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	X	2991	1/1	0.96	0.24	51,51,51,51	0
32	MG	X	3012	1/1	0.96	0.35	45,45,45,45	0
32	MG	X	2938	1/1	0.96	0.21	34,34,34,34	0
32	MG	X	3015	1/1	0.96	0.31	77,77,77,77	0
32	MG	X	2930	1/1	0.96	0.26	51,51,51,51	0
32	MG	C	206	1/1	0.96	0.19	37,37,37,37	0
32	MG	X	2949	1/1	0.96	0.21	48,48,48,48	0
32	MG	X	2889	1/1	0.96	0.16	26,26,26,26	0
33	NA	X	3068	1/1	0.96	0.26	64,64,64,64	0
32	MG	X	2888	1/1	0.96	0.41	36,36,36,36	0
34	K	M	167	1/1	0.96	0.17	44,44,44,44	0
32	MG	X	3025	1/1	0.97	0.10	62,62,62,62	0
32	MG	X	2962	1/1	0.97	0.12	70,70,70,70	0
32	MG	X	2922	1/1	0.97	0.12	19,19,19,19	0
32	MG	X	2905	1/1	0.97	0.22	57,57,57,57	0
32	MG	X	3008	1/1	0.97	0.13	45,45,45,45	0
32	MG	X	3009	1/1	0.97	0.20	53,53,53,53	0
33	NA	X	3051	1/1	0.97	0.12	43,43,43,43	0
32	MG	X	2990	1/1	0.97	0.15	31,31,31,31	0
32	MG	X	2893	1/1	0.97	0.37	25,25,25,25	0
34	K	X	3071	1/1	0.97	0.25	86,86,86,86	0
32	MG	X	2912	1/1	0.97	0.18	24,24,24,24	0
32	MG	X	3013	1/1	0.97	0.14	60,60,60,60	0
32	MG	X	2950	1/1	0.97	0.15	49,49,49,49	0
32	MG	X	2994	1/1	0.97	0.05	41,41,41,41	0
32	MG	X	2958	1/1	0.97	0.04	29,29,29,29	0
32	MG	X	2996	1/1	0.97	0.07	42,42,42,42	0
32	MG	X	2969	1/1	0.97	0.11	31,31,31,31	0
32	MG	X	2998	1/1	0.97	0.19	29,29,29,29	0
32	MG	X	2970	1/1	0.97	0.22	51,51,51,51	0
32	MG	X	2959	1/1	0.97	0.25	33,33,33,33	0
32	MG	X	2960	1/1	0.97	0.19	33,33,33,33	0
32	MG	X	3002	1/1	0.97	0.12	34,34,34,34	0
32	MG	X	2909	1/1	0.97	0.27	44,44,44,44	0
32	MG	X	2886	1/1	0.98	0.17	16,16,16,16	0
32	MG	X	2929	1/1	0.98	0.14	10,10,10,10	0
32	MG	X	2926	1/1	0.98	0.15	35,35,35,35	0
32	MG	X	2894	1/1	0.98	0.13	33,33,33,33	0
32	MG	X	2980	1/1	0.98	0.12	42,42,42,42	0
32	MG	X	2946	1/1	0.98	0.32	38,38,38,38	0
32	MG	X	3006	1/1	0.98	0.10	59,59,59,59	0
32	MG	X	2953	1/1	0.98	0.13	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	X	2936	1/1	0.98	0.15	26,26,26,26	0
32	MG	X	3027	1/1	0.98	0.13	51,51,51,51	0
33	NA	X	3045	1/1	0.98	0.29	31,31,31,31	0
32	MG	X	2890	1/1	0.99	0.24	38,38,38,38	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.