Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:05 am BST

PDB ID	:	2UXC
Title	:	Crystal structure of an extended tRNA anticodon stem loop in complex with its cognate mRNA UCGU in the context of the Thermus thermophilus 30S subunit.
Authors	:	Dunham, C.M.; Selmer, M.; Phelps, S.S.; Kelley, A.C.; Suzuki, T.; Joseph, S.; Ramakrishnan, V.
Deposited on	:	2007-03-28
Resolution	:	2.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

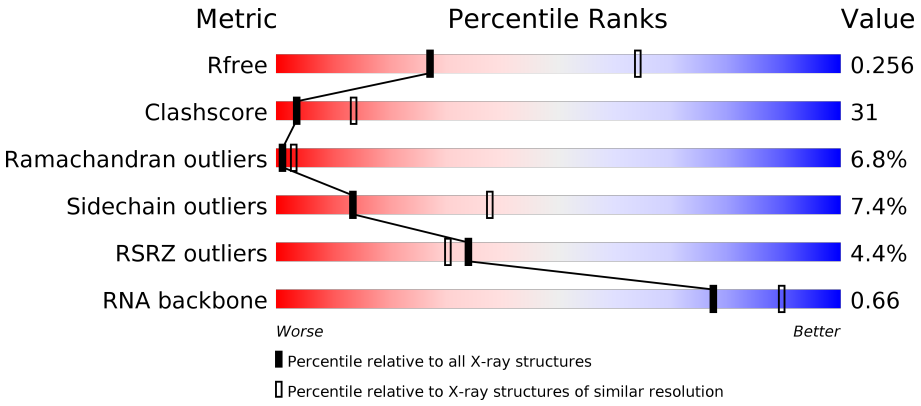
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	4% 36% 50% 11%
2	B	256	7% 23% 57% 11% 8%
3	C	239	5% 23% 51% 12% 13%
4	D	209	5% 51% 42% 7%

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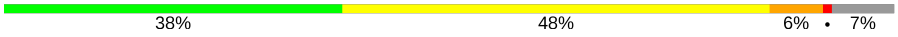
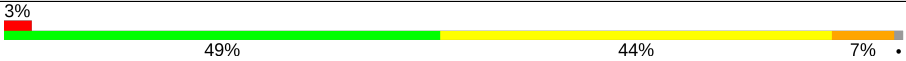
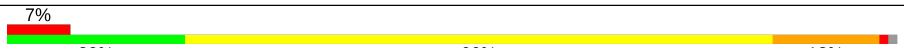
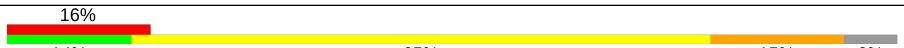
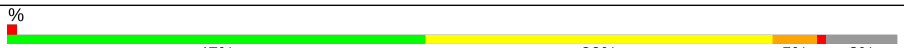
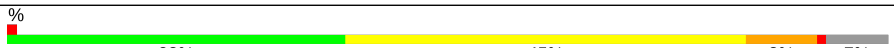
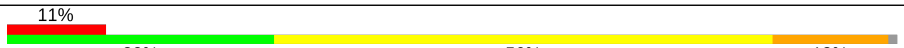
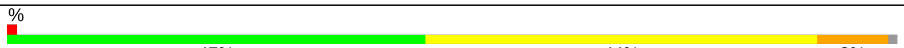
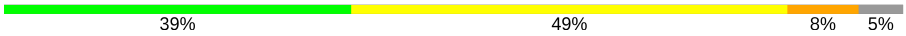
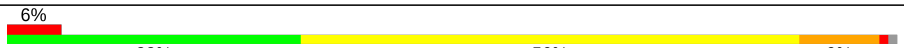
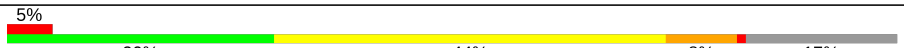
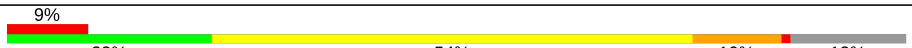
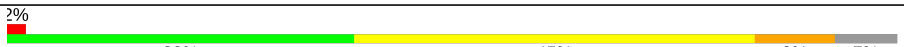
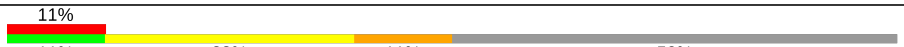
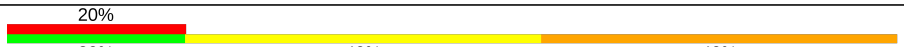
Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	X	18	
23	Y	5	

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
25	MG	A	2023	-	-	-	X
25	MG	A	2025	-	-	-	X
25	MG	A	2125	-	-	-	X
25	MG	A	2148	-	-	-	X
25	MG	A	2184	-	-	-	X

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 52278 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 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1513	32514	14472	6016	10513	1513	0	0	0

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	235	1901	1213	342	341	5	0	0	1

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	207	1613	1016	315	281	1	0	0	1

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	208	1703	1066	339	291	7	0	0	0

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	151	1147	724	218	201	4	0	0	1

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	101	843	531	155	154	3	0	0	0

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	58	ARG	HIS	conflict	UNP P80374

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	41	VAL	ILE	conflict	UNP P80380

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

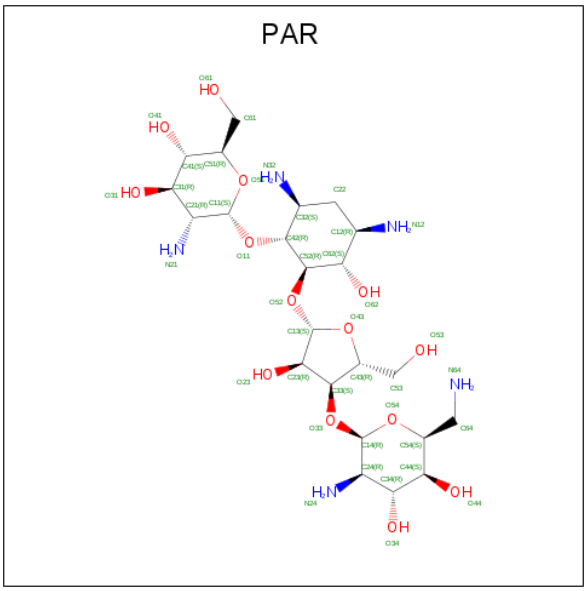
- Molecule 22 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT CGGG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	9	Total	C	N	O	P	0	0	0
			177	81	30	58	8			

- Molecule 23 is a RNA chain called ANTICODON STEM-LOOP OF TRANSFER RNA WITH ANTICODON ACGA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	5	Total	C	N	O	P	0	0	0
			88	37	12	34	5			

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C N O 42 23 5 14	0	0

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	192	Total Mg 192 192	0	0

- Molecule 26 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	26	Total K 26 26	0	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

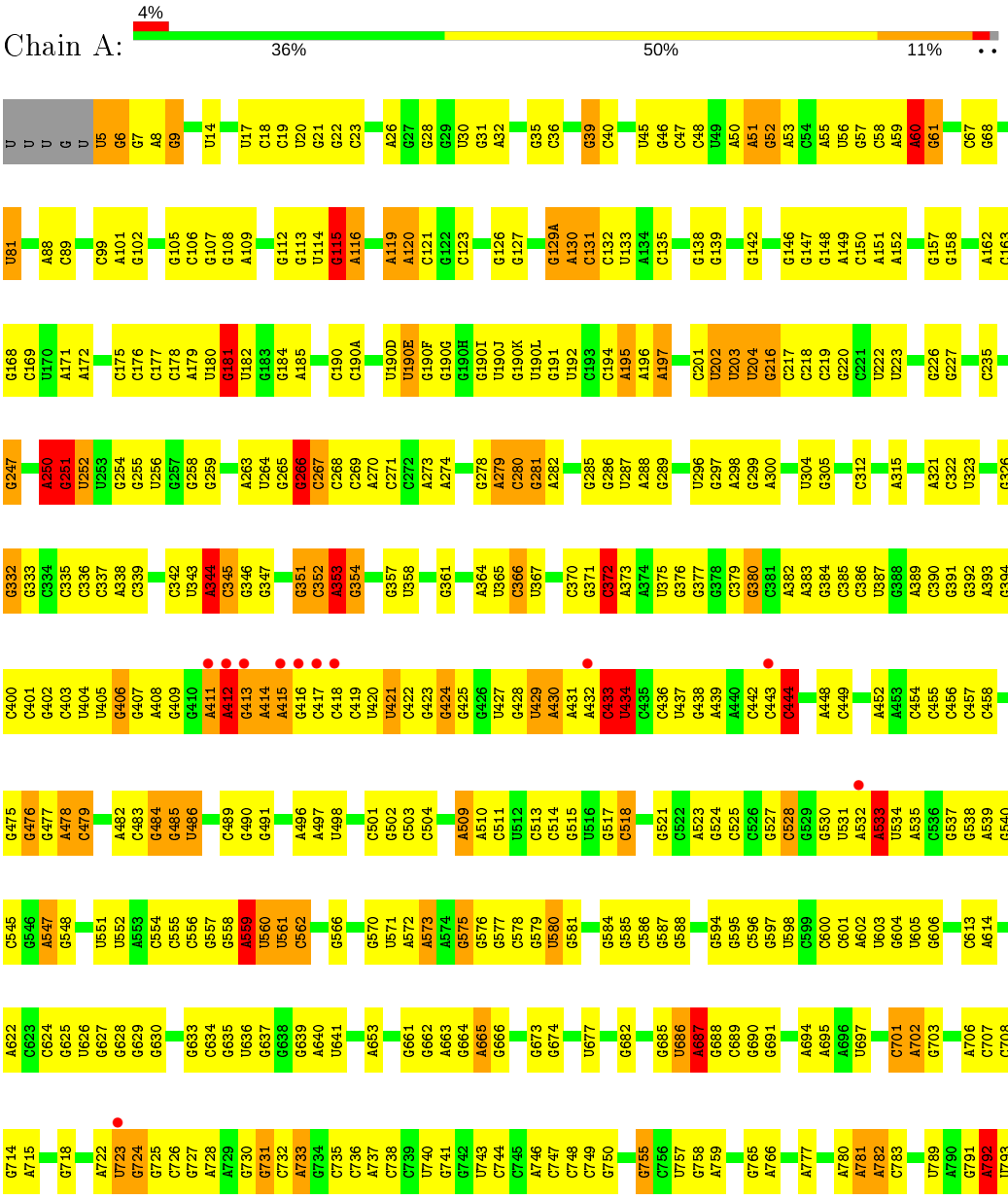
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	2	Total Zn 2 2	0	0

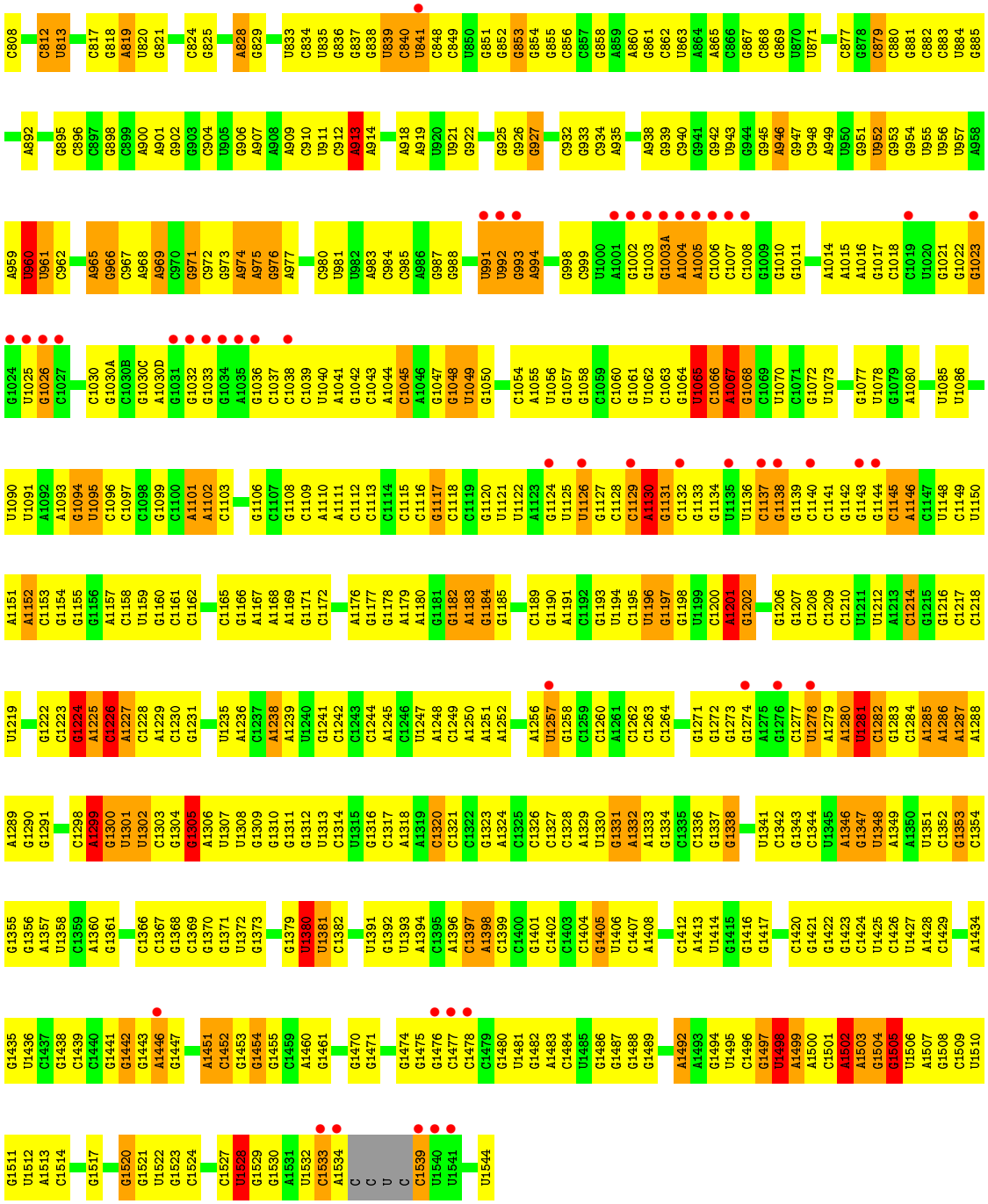
3 Residue-property plots (i)

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

- Molecule 1: 16S RIBOSOMAL RNA

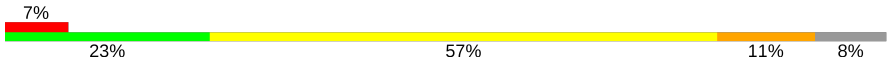
Chain A:

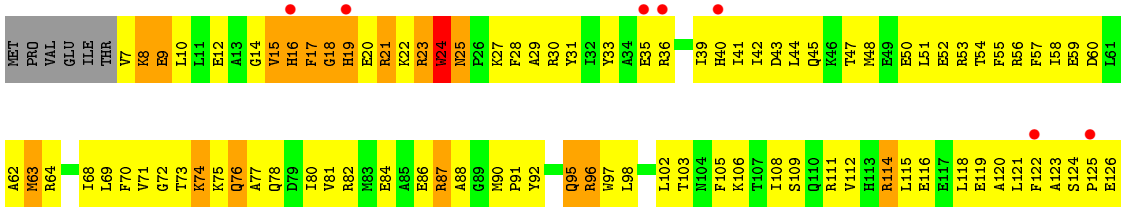


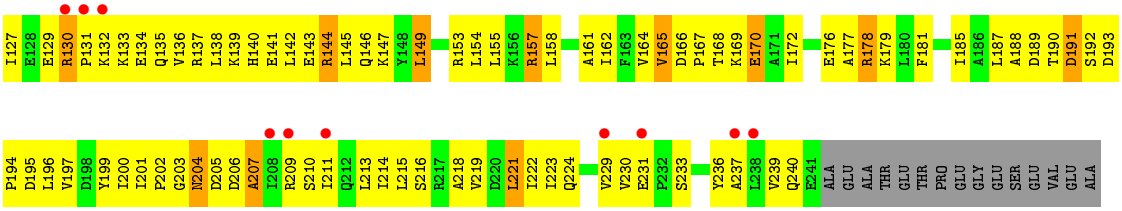


• Molecule 2: RIBOSOMAL PROTEIN S2

Chain B:

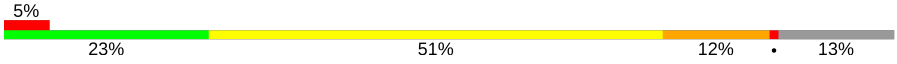


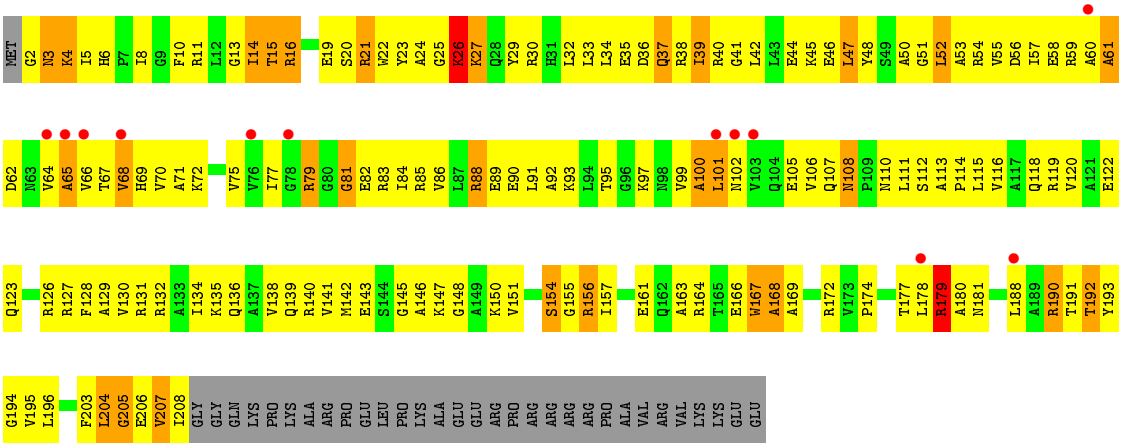




• Molecule 3: RIBOSOMAL PROTEIN S3

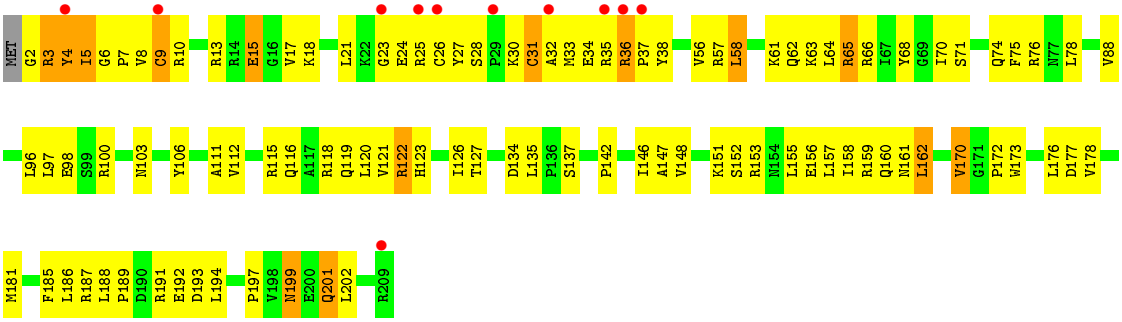
Chain C:





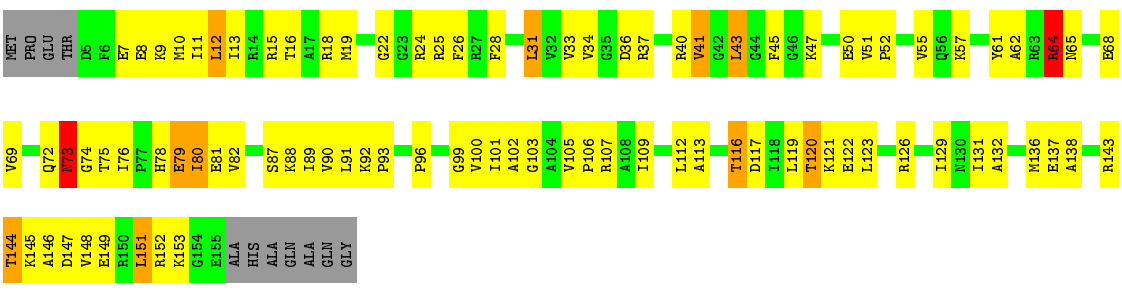
• Molecule 4: RIBOSOMAL PROTEIN S4

Chain D:



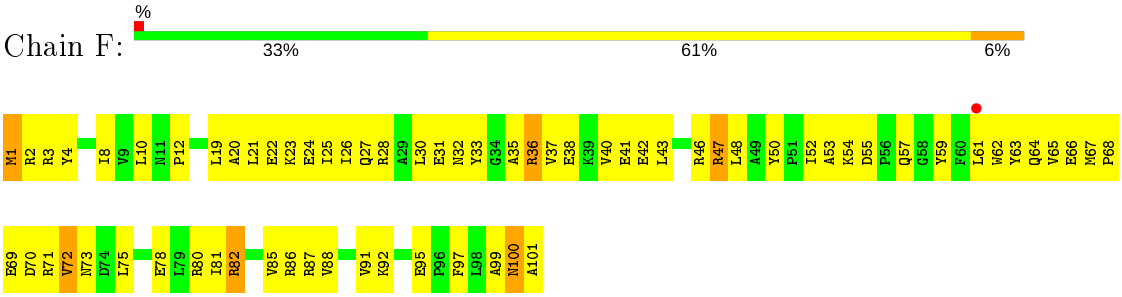
• Molecule 5: RIBOSOMAL PROTEIN S5

Chain E:



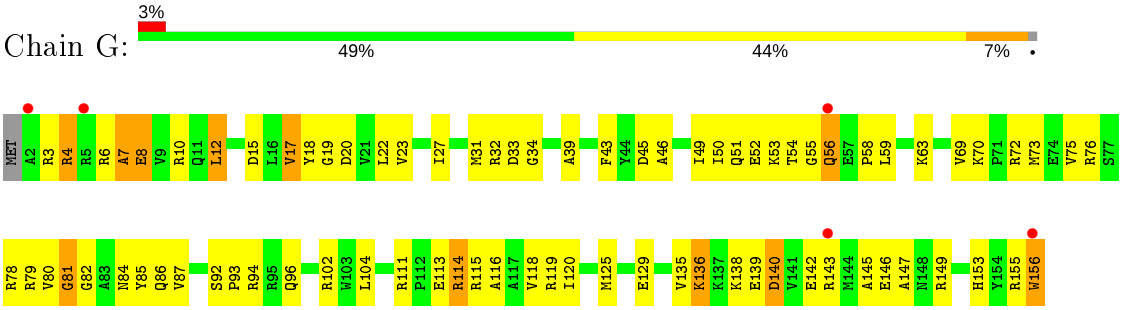
• Molecule 6: RIBOSOMAL PROTEIN S6

Chain F:



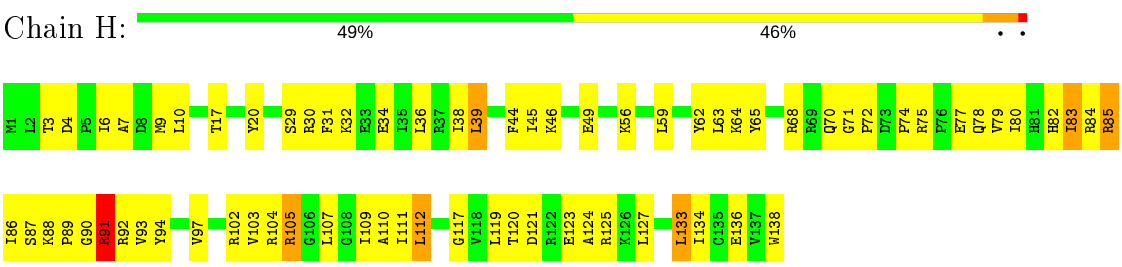
• Molecule 7: RIBOSOMAL PROTEIN S7

Chain G:



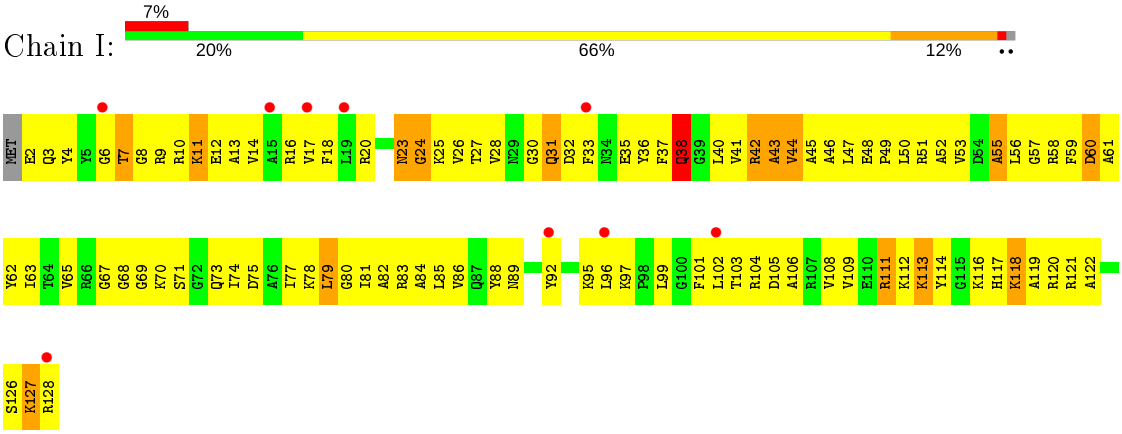
• Molecule 8: RIBOSOMAL PROTEIN S8

Chain H:



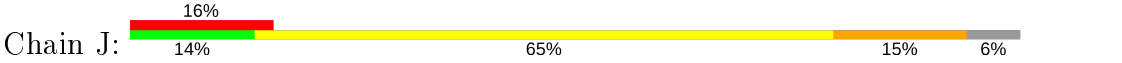
• Molecule 9: RIBOSOMAL PROTEIN S9

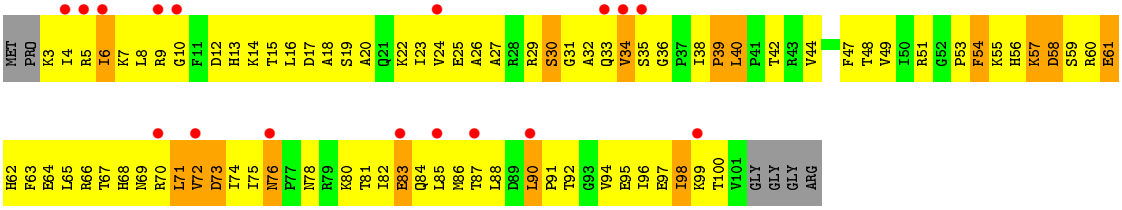
Chain I:



• Molecule 10: RIBOSOMAL PROTEIN S10

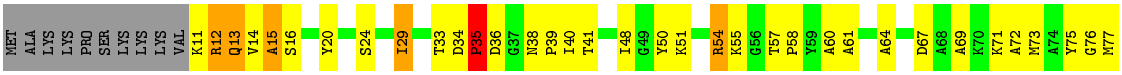
Chain J:

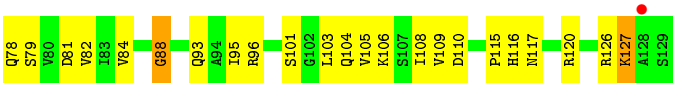




• Molecule 11: RIBOSOMAL PROTEIN S11

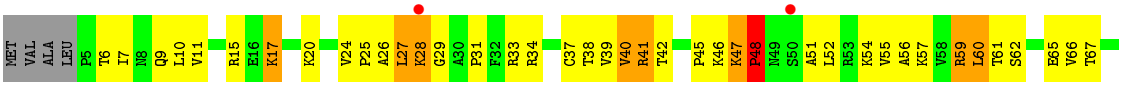
Chain K:





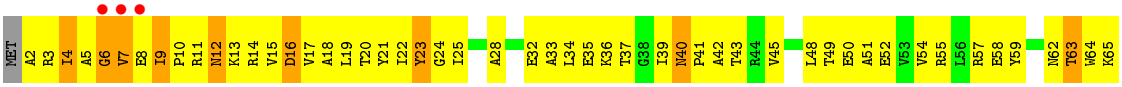
• Molecule 12: RIBOSOMAL PROTEIN S12

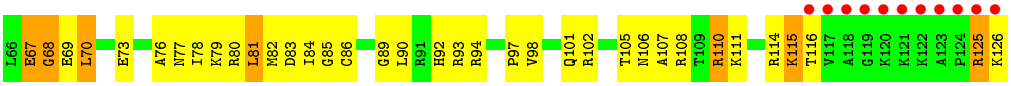
Chain L:



• Molecule 13: RIBOSOMAL PROTEIN S13

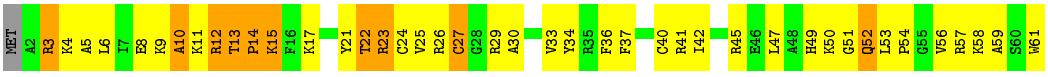
Chain M:





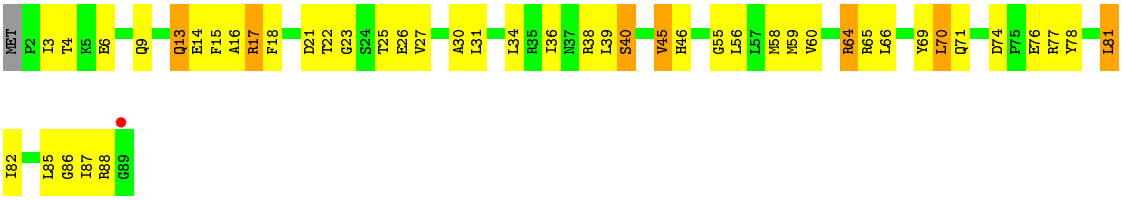
• Molecule 14: RIBOSOMAL PROTEIN S14

Chain N:



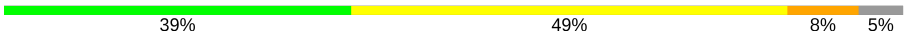
• Molecule 15: RIBOSOMAL PROTEIN S15

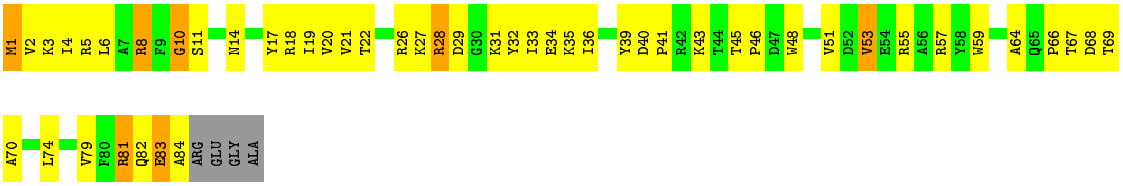
Chain O:



• Molecule 16: RIBOSOMAL PROTEIN S16

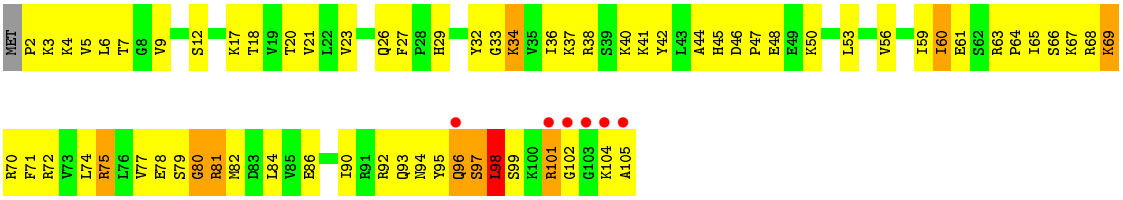
Chain P:





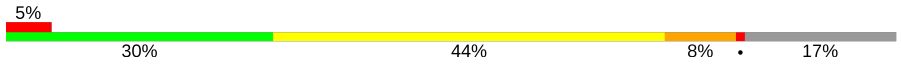
• Molecule 17: RIBOSOMAL PROTEIN S17

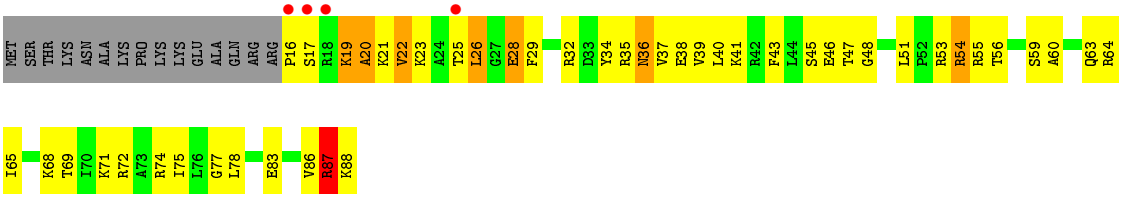
Chain Q:



• Molecule 18: RIBOSOMAL PROTEIN S18

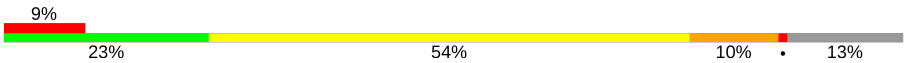
Chain R:

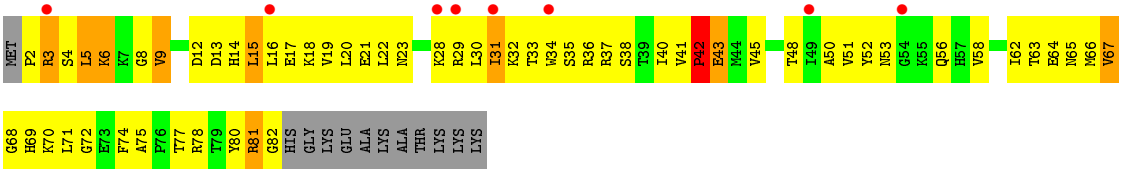




• Molecule 19: RIBOSOMAL PROTEIN S19

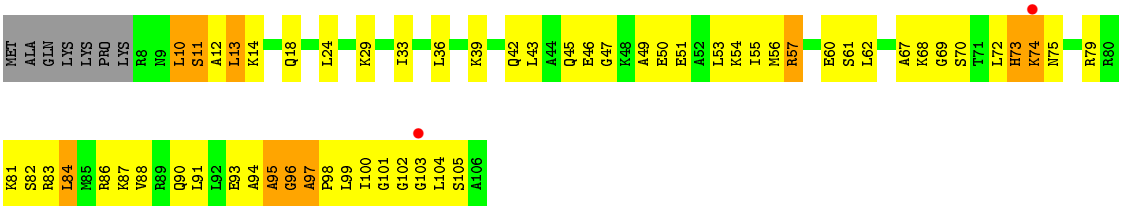
Chain S:





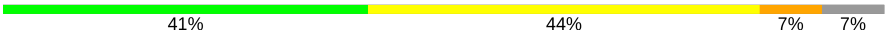
• Molecule 20: RIBOSOMAL PROTEIN S20

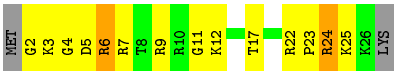
Chain T:



• Molecule 21: RIBOSOMAL PROTEIN THX

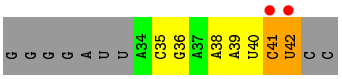
Chain U:





• Molecule 22: A-SITE MESSENGER RNA FRAGMENT CGGG

Chain X:



• Molecule 23: ANTICODON STEM-LOOP OF TRANSFER RNA WITH ANTICODON ACGA

Chain Y:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	401.82Å 401.82Å 175.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.28 – 2.90 48.28 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.28-2.90) 97.5 (48.28-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.255 0.218 , 0.256	Depositor DCC
R_{free} test set	15260 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	67.7	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 73.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	52278	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.47	0/36394	0.74	39/56801 (0.1%)
2	B	0.34	0/1936	0.61	0/2611
3	C	0.37	0/1637	0.62	0/2207
4	D	0.34	0/1733	0.60	0/2318
5	E	0.46	0/1163	0.73	1/1566 (0.1%)
6	F	0.30	0/856	0.61	0/1154
7	G	0.32	0/1276	0.54	0/1709
8	H	0.46	0/1136	0.76	0/1527
9	I	0.34	0/1029	0.64	1/1378 (0.1%)
10	J	0.37	0/806	0.67	0/1084
11	K	0.35	0/900	0.66	0/1213
12	L	0.43	0/987	0.75	0/1322
13	M	0.33	0/1008	0.62	0/1347
14	N	0.39	0/501	0.66	0/664
15	O	0.37	0/745	0.64	1/992 (0.1%)
16	P	0.43	0/717	0.74	0/965
17	Q	0.41	0/870	0.76	0/1159
18	R	0.32	0/603	0.57	0/799
19	S	0.35	0/662	0.67	0/892
20	T	0.40	0/764	0.70	0/1006
21	U	0.51	0/213	0.64	0/279
22	X	0.37	0/197	0.70	0/305
23	Y	1.04	2/96 (2.1%)	0.82	0/146
All	All	0.44	2/56229 (0.0%)	0.71	42/83444 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	33

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	1	U	OP3-P	-6.74	1.53	1.61
23	Y	1	U	P-O5'	5.15	1.64	1.59

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	243	A	C2'-C3'-O3'	9.37	130.11	109.50
1	A	281	G	C2'-C3'-O3'	9.23	129.81	109.50
1	A	115	G	C2'-C3'-O3'	9.12	129.56	109.50
1	A	366	C	C2'-C3'-O3'	8.84	128.94	109.50
1	A	1498	U	C2'-C3'-O3'	8.81	128.87	109.50
1	A	559	A	C2'-C3'-O3'	8.58	128.37	109.50
1	A	1528	U	C2'-C3'-O3'	8.54	128.29	109.50
1	A	181	G	C2'-C3'-O3'	8.48	128.16	109.50
1	A	1302	U	C2'-C3'-O3'	8.21	127.57	109.50
1	A	687	A	C2'-C3'-O3'	7.93	126.94	109.50
1	A	328	C	C2'-C3'-O3'	7.88	126.83	109.50
1	A	60	A	C2'-C3'-O3'	7.53	126.07	109.50
1	A	266	G	C2'-C3'-O3'	7.28	125.52	109.50
1	A	792	A	C2'-C3'-O3'	7.18	125.29	109.50
1	A	533	A	C2'-C3'-O3'	7.13	125.19	109.50
1	A	1299	A	N9-C1'-C2'	7.02	123.13	114.00
1	A	1505	G	C2'-C3'-O3'	6.84	124.64	113.70
1	A	1201	A	C2'-C3'-O3'	6.80	124.58	113.70
1	A	484	G	C2'-C3'-O3'	6.75	124.50	113.70
1	A	965	A	C2'-C3'-O3'	6.64	124.33	113.70
1	A	509	A	C2'-C3'-O3'	6.48	124.07	113.70
1	A	1502	A	N9-C1'-C2'	6.41	122.34	114.00
1	A	433	C	N1-C1'-C2'	6.38	122.29	114.00
1	A	1380	U	C2'-C3'-O3'	6.32	123.81	113.70
15	O	45	VAL	N-CA-C	-6.30	93.98	111.00
1	A	792	A	C4'-C3'-O3'	-6.23	96.31	109.40
1	A	1380	U	N1-C1'-C2'	6.17	122.02	114.00
1	A	913	A	C2'-C3'-O3'	6.14	123.53	113.70
1	A	372	C	C2'-C3'-O3'	6.03	123.36	113.70
1	A	1065	U	C1'-O4'-C4'	-5.93	105.15	109.90
1	A	1528	U	C4'-C3'-O3'	5.86	124.73	113.00
1	A	353	A	C5'-C4'-O4'	-5.77	102.17	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	60	ASP	N-CA-C	-5.75	95.46	111.00
5	E	64	ARG	N-CA-C	-5.73	95.54	111.00
1	A	1305	G	N9-C1'-C2'	5.71	121.42	114.00
1	A	960	U	C2'-C3'-O3'	5.52	122.53	113.70
1	A	1224	G	C2'-C3'-O3'	5.34	122.25	113.70
1	A	412	A	N9-C1'-C2'	5.26	120.83	114.00
1	A	444	C	N1-C1'-C2'	5.25	120.82	114.00
1	A	434	U	N1-C1'-C2'	5.14	120.68	114.00
1	A	1067	A	C2'-C3'-O3'	5.13	121.91	113.70
1	A	281	G	C4'-C3'-O3'	5.04	123.07	113.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	243	A	C3'
1	A	281	G	C3'
1	A	366	C	C3'
1	A	1528	U	C3'

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1048	G	Sidechain
1	A	1077	G	Sidechain
1	A	1130	A	Sidechain
1	A	1226	C	Sidechain
1	A	1281	U	Sidechain
1	A	1299	A	Sidechain
1	A	14	U	Sidechain
1	A	1405	G	Sidechain
1	A	1454	G	Sidechain
1	A	1492	A	Sidechain
1	A	1498	U	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	297	G	Sidechain
1	A	344	A	Sidechain
1	A	380	G	Sidechain
1	A	433	C	Sidechain
1	A	528	C	Sidechain
1	A	545	C	Sidechain
1	A	561	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	573	A	Sidechain
1	A	580	U	Sidechain
1	A	587	G	Sidechain
1	A	682	G	Sidechain
1	A	691	G	Sidechain
1	A	697	U	Sidechain
1	A	727	G	Sidechain
1	A	853	G	Sidechain
1	A	871	U	Sidechain
1	A	879	C	Sidechain
1	A	898	G	Sidechain
1	A	946	A	Sidechain
1	A	952	U	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32514	0	16411	1016	0
2	B	1901	0	1951	244	0
3	C	1613	0	1677	247	0
4	D	1703	0	1764	117	0
5	E	1147	0	1207	107	0
6	F	843	0	857	84	0
7	G	1257	0	1296	90	0
8	H	1116	0	1177	77	0
9	I	1011	0	1043	129	0
10	J	793	0	835	162	0
11	K	885	0	904	60	0
12	L	971	0	1057	105	0
13	M	997	0	1072	113	0
14	N	492	0	529	69	0
15	O	734	0	771	48	0
16	P	701	0	720	59	0
17	Q	857	0	930	80	0
18	R	597	0	666	74	0
19	S	648	0	673	79	0
20	T	762	0	859	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	U	209	0	221	24	0
22	X	177	0	91	9	0
23	Y	88	0	42	8	0
24	A	42	0	45	1	0
25	A	192	0	0	0	0
26	A	26	0	0	0	0
27	A	2	0	0	0	0
All	All	52278	0	36798	2801	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 31.

All (2801) 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)
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.21	1.19
22:X:41:C:H2'	22:X:42:U:H4'	1.24	1.18
1:A:478:A:H2'	1:A:479:C:H5'	1.26	1.16
12:L:41:ARG:HG2	12:L:42:THR:H	1.17	1.10
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.33	1.10
2:B:16:HIS:HA	2:B:204:ASN:HD21	1.10	1.10
3:C:3:ASN:N	3:C:3:ASN:HD22	1.45	1.09
4:D:151:LYS:H	4:D:151:LYS:HD2	1.15	1.08
1:A:1443:G:H5"	1:A:1446:A:H5'	1.34	1.05
6:F:33:TYR:HA	6:F:71:ARG:HH21	1.16	1.04
1:A:243:A:H4'	1:A:244:U:H5'	1.38	1.03
21:U:9:ARG:HH12	21:U:23:PRO:HD2	1.20	1.02
18:R:47:THR:HG22	18:R:48:GLY:H	1.18	1.02
9:I:108:VAL:HG12	9:I:109:VAL:H	1.25	1.01
1:A:877:C:O2	8:H:3:THR:HG21	1.60	1.01
23:Y:3:G:H2'	23:Y:4:U:H5"	1.39	1.01
10:J:34:VAL:HG13	10:J:74:ILE:HA	1.43	1.00
3:C:34:LEU:HD12	14:N:25:VAL:HG21	1.42	1.00
1:A:1060:C:C5	3:C:2:GLY:HA3	1.97	1.00
3:C:26:LYS:HE2	3:C:26:LYS:N	1.76	1.00
10:J:4:ILE:HD12	10:J:74:ILE:HB	1.41	1.00
19:S:15:LEU:HA	19:S:18:LYS:HB3	1.44	1.00
10:J:32:ALA:HB3	10:J:75:ILE:HG23	1.44	0.99
1:A:477:G:H2'	1:A:478:A:H5"	1.44	0.98
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.28	0.98
12:L:47:LYS:HB3	12:L:48:PRO:CD	1.95	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.44	0.97
1:A:1086:U:H3	1:A:1099:G:H22	1.09	0.96
2:B:16:HIS:HA	2:B:204:ASN:ND2	1.79	0.96
13:M:49:THR:HB	13:M:52:GLU:HG3	1.47	0.96
1:A:414:A:H8	1:A:416:G:H1	1.08	0.95
17:Q:53:LEU:H	17:Q:53:LEU:HD12	1.30	0.95
2:B:161:ALA:HB1	2:B:185:ILE:HD11	1.49	0.94
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.48	0.94
1:A:266:G:H5"	1:A:268:C:H41	1.32	0.94
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.49	0.94
1:A:412:A:O2'	1:A:413:G:H5"	1.69	0.93
10:J:90:LEU:H	10:J:91:PRO:HD2	1.32	0.93
1:A:1057:G:H5"	3:C:154:SER:HB2	1.51	0.92
2:B:102:LEU:HD21	2:B:162:ILE:HD11	1.52	0.92
1:A:1226:C:H4'	1:A:1227:A:OP1	1.71	0.91
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.52	0.91
3:C:108:ASN:HD22	3:C:111:LEU:HG	1.35	0.91
3:C:3:ASN:HD22	3:C:3:ASN:H	1.18	0.91
6:F:47:ARG:HE	6:F:47:ARG:H	1.17	0.91
1:A:431:A:H2'	1:A:433:C:N4	1.86	0.90
2:B:69:LEU:HD12	2:B:155:LEU:HD11	1.53	0.90
1:A:412:A:C4	1:A:413:G:H2'	2.06	0.90
1:A:972:C:H4'	10:J:57:LYS:HG2	1.51	0.90
17:Q:97:SER:HA	17:Q:102:GLY:HA2	1.50	0.90
1:A:414:A:H2'	1:A:416:G:N2	1.85	0.90
1:A:1137:C:H4'	1:A:1138:G:C2	2.06	0.90
1:A:1250:A:H4'	9:I:68:GLY:H	1.37	0.90
3:C:64:VAL:HB	3:C:99:VAL:HG21	1.52	0.90
11:K:54:ARG:O	11:K:57:THR:HG22	1.71	0.90
1:A:1369:C:H2'	1:A:1370:G:C8	2.07	0.89
13:M:8:GLU:HG3	13:M:22:ILE:HG23	1.53	0.89
19:S:33:THR:HG22	19:S:35:SER:H	1.35	0.89
15:O:88:ARG:HB2	15:O:88:ARG:NH1	1.88	0.89
20:T:50:GLU:H	20:T:99:LEU:HD12	1.35	0.89
3:C:26:LYS:H	3:C:26:LYS:HE2	1.38	0.89
18:R:86:VAL:O	18:R:87:ARG:HB2	1.71	0.89
6:F:47:ARG:NE	6:F:47:ARG:H	1.71	0.88
20:T:57:ARG:HH11	20:T:57:ARG:HB2	1.38	0.88
1:A:664:G:H22	1:A:741:G:H1	1.20	0.88
9:I:127:LYS:HD2	9:I:127:LYS:H	1.38	0.88
1:A:1238:A:H5'	1:A:1336:C:H41	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.55	0.88
9:I:70:LYS:O	9:I:74:ILE:HG13	1.74	0.88
1:A:1367:C:H5'	10:J:60:ARG:NH1	1.88	0.88
20:T:45:GLN:HB2	20:T:91:LEU:HD13	1.55	0.87
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.54	0.87
18:R:19:LYS:HD2	18:R:20:ALA:H	1.39	0.87
3:C:131:ARG:HG2	3:C:135:LYS:HE3	1.57	0.87
1:A:1124:G:H5'	10:J:35:SER:O	1.75	0.87
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.57	0.86
23:Y:3:G:C2'	23:Y:4:U:H5"	2.05	0.86
1:A:1502:A:H2	1:A:1505:G:H1	1.23	0.86
1:A:838:G:H2'	1:A:839:U:H5"	1.54	0.86
12:L:55:VAL:HG12	12:L:56:ALA:H	1.38	0.86
5:E:144:THR:HG22	5:E:147:ASP:H	1.41	0.86
1:A:1125:U:H3	10:J:5:ARG:HH21	1.23	0.86
1:A:328:C:O2	1:A:328:C:H2'	1.74	0.86
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.57	0.86
10:J:49:VAL:HG13	14:N:41:ARG:HD2	1.58	0.86
1:A:478:A:C2'	1:A:479:C:H5'	2.04	0.85
2:B:19:HIS:CE1	2:B:204:ASN:HB3	2.11	0.85
10:J:90:LEU:H	10:J:91:PRO:CD	1.89	0.85
3:C:172:ARG:HH12	3:C:174:PRO:HG3	1.41	0.85
1:A:1366:C:H2'	1:A:1367:C:H6	1.41	0.85
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.59	0.85
1:A:1305:G:HO2'	1:A:1306:A:H8	1.21	0.84
2:B:16:HIS:CA	2:B:204:ASN:HD21	1.88	0.84
1:A:1250:A:H4'	9:I:68:GLY:N	1.93	0.84
1:A:1006:C:H2'	1:A:1007:C:H6	1.41	0.84
3:C:14:ILE:HG22	3:C:15:THR:H	1.42	0.84
3:C:48:TYR:HA	3:C:52:LEU:HD22	1.59	0.84
7:G:54:THR:HG22	7:G:55:GLY:H	1.40	0.84
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.56	0.84
1:A:112:G:H21	1:A:354:G:H5'	1.43	0.84
1:A:1347:G:H3'	9:I:108:VAL:O	1.78	0.84
21:U:24:ARG:HB3	21:U:24:ARG:HH11	1.41	0.84
2:B:18:GLY:HA2	2:B:41:ILE:HA	1.60	0.84
1:A:1391:U:H2'	1:A:1392:G:C8	2.12	0.83
1:A:706:A:C1'	11:K:29:ILE:HD11	2.08	0.83
1:A:414:A:H2'	1:A:416:G:C2	2.12	0.83
2:B:23:ARG:NH1	2:B:191:ASP:HA	1.93	0.83
3:C:191:THR:HG22	3:C:193:TYR:H	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:U:HO2'	1:A:687:A:H8	1.22	0.83
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.18	0.83
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.60	0.82
5:E:80:ILE:CD1	5:E:91:LEU:HB2	2.09	0.82
2:B:178:ARG:HG3	2:B:178:ARG:HH11	1.41	0.82
10:J:20:ALA:O	10:J:24:VAL:HG23	1.79	0.82
13:M:15:VAL:HG23	13:M:43:THR:O	1.79	0.82
1:A:1443:G:H5"	1:A:1446:A:C5'	2.07	0.82
1:A:1347:G:N2	1:A:1373:G:H2'	1.93	0.82
14:N:26:ARG:NE	14:N:47:LEU:HD21	1.94	0.82
1:A:1189:C:P	10:J:51:ARG:HH22	2.02	0.82
22:X:41:C:H2'	22:X:42:U:C4'	2.09	0.82
1:A:1038:C:H2'	1:A:1039:C:H6	1.44	0.82
3:C:52:LEU:HD21	3:C:118:GLN:HE22	1.45	0.81
1:A:351:G:H4'	1:A:352:C:OP1	1.79	0.81
10:J:27:ALA:HA	10:J:81:THR:HG23	1.61	0.81
1:A:1101:A:H4'	1:A:1102:A:O5'	1.80	0.81
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.61	0.81
1:A:371:G:O2'	1:A:372:C:H5'	1.79	0.81
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.62	0.81
14:N:57:ARG:HG2	14:N:58:LYS:H	1.45	0.81
1:A:738:C:OP2	6:F:92:LYS:HE3	1.80	0.81
1:A:1103:C:H5"	2:B:98:LEU:HD12	1.63	0.81
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.61	0.81
1:A:1443:G:C5'	1:A:1446:A:H5'	2.11	0.81
3:C:3:ASN:N	3:C:3:ASN:ND2	2.20	0.81
2:B:130:ARG:HB3	2:B:131:PRO:HD2	1.62	0.80
1:A:559:A:P	5:E:126:ARG:HH22	2.04	0.80
13:M:49:THR:HG22	13:M:51:ALA:H	1.47	0.80
19:S:64:GLU:O	19:S:67:VAL:HG23	1.80	0.80
1:A:202:U:H5"	1:A:203:U:OP2	1.81	0.80
1:A:1038:C:H2'	1:A:1039:C:C6	2.16	0.80
1:A:418:C:H5'	1:A:539:A:O2'	1.80	0.80
10:J:64:GLU:HB3	14:N:59:ALA:HB2	1.62	0.80
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.63	0.80
2:B:73:THR:HG23	2:B:96:ARG:HH21	1.46	0.80
14:N:9:LYS:HD3	14:N:10:ALA:N	1.96	0.80
10:J:4:ILE:HA	10:J:100:THR:HA	1.63	0.80
11:K:54:ARG:NH1	11:K:54:ARG:HB3	1.97	0.80
1:A:1281:U:H5'	1:A:1282:C:H5	1.45	0.79
19:S:17:GLU:HA	19:S:20:LEU:HG	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:G:H4'	9:I:126:SER:HB2	1.64	0.79
1:A:477:G:C2'	1:A:478:A:H5"	2.12	0.79
20:T:57:ARG:HH22	20:T:100:ILE:HD11	1.46	0.79
16:P:81:ARG:HE	16:P:83:GLU:HG3	1.47	0.79
1:A:839:U:H5'	1:A:840:C:H5	1.46	0.79
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.18	0.79
1:A:1305:G:O2'	1:A:1306:A:H8	1.65	0.79
6:F:22:GLU:OE1	6:F:82:ARG:HD3	1.83	0.79
7:G:4:ARG:HB3	7:G:4:ARG:HH11	1.48	0.79
1:A:1086:U:H3	1:A:1099:G:N2	1.81	0.79
2:B:80:ILE:H	2:B:80:ILE:HD12	1.46	0.79
7:G:146:GLU:HG2	7:G:149:ARG:HH21	1.47	0.79
1:A:1003(A):G:H2'	1:A:1004:A:H4'	1.65	0.78
10:J:19:SER:HA	10:J:22:LYS:HZ3	1.47	0.78
10:J:10:GLY:H	10:J:16:LEU:HD11	1.48	0.78
10:J:39:PRO:O	10:J:40:LEU:HB2	1.83	0.78
1:A:840:C:H5'	1:A:848:C:O2	1.84	0.78
6:F:80:ARG:HH11	6:F:88:VAL:HB	1.49	0.78
7:G:56:GLN:H	7:G:56:GLN:CD	1.86	0.78
18:R:17:SER:HB2	18:R:54:ARG:NH2	1.99	0.78
1:A:1366:C:H2'	1:A:1367:C:C6	2.19	0.78
10:J:34:VAL:HA	10:J:75:ILE:HG22	1.66	0.78
1:A:933:G:OP1	7:G:4:ARG:HD2	1.85	0.77
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.20	0.77
12:L:75:HIS:HD2	12:L:77:LEU:H	1.31	0.77
1:A:1532:U:O2'	1:A:1533:C:H4'	1.83	0.77
18:R:47:THR:HG22	18:R:48:GLY:N	1.97	0.77
1:A:250:A:H4'	1:A:251:G:O5'	1.82	0.77
13:M:54:VAL:O	13:M:58:GLU:HG2	1.83	0.77
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.66	0.77
1:A:412:A:H1'	1:A:413:G:H2'	1.66	0.77
2:B:143:GLU:O	2:B:147:LYS:HG3	1.84	0.77
19:S:53:ASN:HD21	19:S:56:GLN:HB2	1.49	0.77
1:A:677:U:H3	1:A:713:G:H22	1.32	0.77
1:A:969:A:H61	13:M:126:LYS:HB3	1.50	0.77
2:B:134:GLU:HG2	2:B:137:ARG:NH2	2.00	0.77
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.66	0.77
1:A:686:U:O2'	1:A:687:A:H8	1.68	0.77
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.67	0.77
12:L:59:ARG:NH2	12:L:65:GLU:HB3	2.00	0.77
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:62:ASN:O	13:M:63:THR:HB	1.84	0.76
4:D:62:GLN:HA	4:D:62:GLN:HE21	1.48	0.76
9:I:127:LYS:HB2	13:M:126:LYS:NZ	2.00	0.76
1:A:175:C:H2'	1:A:176:C:H6	1.51	0.76
1:A:133:U:OP1	20:T:74:LYS:HE2	1.85	0.76
3:C:79:ARG:HH21	3:C:82:GLU:HG2	1.51	0.76
18:R:38:GLU:CD	18:R:38:GLU:H	1.88	0.76
3:C:89:GLU:O	3:C:93:LYS:HG2	1.86	0.76
5:E:149:GLU:O	5:E:153:LYS:HG2	1.86	0.76
19:S:77:THR:HG22	19:S:78:ARG:HG3	1.67	0.76
1:A:243:A:C4'	1:A:244:U:H5'	2.15	0.76
1:A:1190:G:OP1	3:C:4:LYS:HA	1.85	0.76
1:A:839:U:H5'	1:A:840:C:C5	2.20	0.76
17:Q:74:LEU:O	17:Q:75:ARG:HB3	1.86	0.76
20:T:90:GLN:O	20:T:93:GLU:HG2	1.86	0.76
3:C:15:THR:O	3:C:16:ARG:HB2	1.85	0.75
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.68	0.75
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.68	0.75
1:A:967:C:H4'	9:I:128:ARG:HG3	1.67	0.75
1:A:414:A:H61	1:A:427:U:H3	1.31	0.75
2:B:139:LYS:O	2:B:143:GLU:HG2	1.87	0.75
2:B:84:GLU:OE1	2:B:216:SER:HA	1.86	0.75
17:Q:4:LYS:HE3	17:Q:6:LEU:HD21	1.67	0.75
1:A:706:A:H1'	11:K:29:ILE:HD11	1.66	0.75
7:G:140:ASP:HA	7:G:143:ARG:HD2	1.69	0.75
1:A:1369:C:H2'	1:A:1370:G:H8	1.49	0.74
12:L:41:ARG:HG2	12:L:42:THR:N	1.99	0.74
12:L:47:LYS:CB	12:L:48:PRO:HD3	2.11	0.74
3:C:20:SER:O	14:N:54:PRO:HB3	1.87	0.74
2:B:17:PHE:HB3	2:B:44:LEU:HD21	1.69	0.74
3:C:37:GLN:HE22	14:N:52:GLN:HG2	1.53	0.74
17:Q:21:VAL:HG21	17:Q:59:ILE:HD11	1.68	0.74
1:A:975:A:H5'	1:A:975:A:H8	1.52	0.74
3:C:13:GLY:HA3	14:N:57:ARG:HH21	1.51	0.74
3:C:34:LEU:HD23	3:C:34:LEU:C	2.08	0.74
22:X:41:C:C2'	22:X:42:U:H4'	2.14	0.74
1:A:1148:U:H2'	1:A:1149:C:O4'	1.88	0.74
1:A:1080:A:H5"	5:E:16:THR:HG21	1.70	0.73
1:A:35:G:H2'	1:A:36:C:C6	2.23	0.73
4:D:62:GLN:HE22	4:D:65:ARG:NH1	1.86	0.73
11:K:84:VAL:HG22	11:K:110:ASP:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:80:ILE:HD11	5:E:91:LEU:HB2	1.70	0.73
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.70	0.73
1:A:1425:U:H2'	1:A:1426:C:C6	2.22	0.73
1:A:412:A:N9	1:A:413:G:H2'	2.03	0.73
3:C:41:GLY:O	3:C:45:LYS:HG2	1.89	0.73
9:I:97:LYS:HG2	9:I:102:LEU:HD12	1.69	0.73
13:M:4:ILE:HG22	13:M:5:ALA:N	2.04	0.73
10:J:98:ILE:H	10:J:98:ILE:HD12	1.51	0.73
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.18	0.73
2:B:223:ILE:HD12	2:B:224:GLN:N	2.03	0.73
4:D:36:ARG:H	4:D:37:PRO:HD3	1.53	0.73
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.70	0.73
1:A:840:C:H5"	1:A:841:U:OP1	1.88	0.73
1:A:1116:C:C2'	1:A:1117:G:H5"	2.18	0.73
1:A:1057:G:H5"	3:C:154:SER:CB	2.18	0.73
5:E:24:ARG:HH11	5:E:24:ARG:HG2	1.54	0.73
1:A:1006:C:H2'	1:A:1007:C:C6	2.22	0.73
17:Q:68:ARG:HH11	17:Q:68:ARG:HG2	1.54	0.73
1:A:1277:C:H2'	1:A:1278:U:H5'	1.71	0.72
1:A:992:U:H4'	1:A:993:G:O5'	1.88	0.72
1:A:1330:U:OP1	13:M:23:TYR:O	2.07	0.72
3:C:10:PHE:CE2	3:C:178:LEU:HD13	2.23	0.72
1:A:939:G:H5"	7:G:102:ARG:NH2	2.03	0.72
1:A:1116:C:H2'	1:A:1117:G:H5"	1.70	0.72
1:A:1182:G:H4'	1:A:1183:A:H5"	1.72	0.72
6:F:100:ASN:HA	18:R:23:LYS:HE3	1.70	0.72
1:A:838:G:C2'	1:A:839:U:H5"	2.19	0.72
4:D:8:VAL:O	4:D:10:ARG:N	2.21	0.72
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.72	0.72
1:A:112:G:H4'	1:A:389:A:H5"	1.71	0.72
8:H:112:LEU:HD23	8:H:112:LEU:N	2.03	0.72
1:A:1222:G:OP1	19:S:77:THR:HG21	1.88	0.72
1:A:1152:A:H5"	10:J:13:HIS:CD2	2.24	0.72
1:A:163:C:O2'	1:A:164:U:H5'	1.89	0.72
1:A:714:G:H2'	1:A:715:A:C8	2.25	0.72
10:J:49:VAL:O	10:J:60:ARG:HA	1.88	0.72
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.72	0.72
3:C:190:ARG:HB3	3:C:190:ARG:HH11	1.55	0.71
4:D:187:ARG:HD2	4:D:188:LEU:H	1.55	0.71
3:C:174:PRO:HB2	3:C:177:THR:CG2	2.20	0.71
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:LYS:O	10:J:57:LYS:HD2	1.89	0.71
18:R:36:ASN:ND2	18:R:38:GLU:HG2	2.06	0.71
1:A:1133:G:H2'	1:A:1134:G:H8	1.55	0.71
1:A:478:A:H2'	1:A:479:C:C5'	2.13	0.71
12:L:28:LYS:HD3	12:L:33:ARG:HH22	1.55	0.71
1:A:1256:A:H5'	1:A:1258:G:H1'	1.73	0.71
9:I:108:VAL:HG12	9:I:109:VAL:N	2.04	0.71
10:J:35:SER:HB2	10:J:72:VAL:O	1.91	0.71
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.24	0.71
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.05	0.71
2:B:59:GLU:HB2	2:B:221:LEU:HD11	1.73	0.71
10:J:42:THR:HG23	10:J:67:THR:O	1.90	0.71
16:P:20:VAL:HG11	16:P:32:TYR:HB3	1.73	0.71
1:A:759:A:H61	17:Q:94:ASN:HD21	1.38	0.71
3:C:91:LEU:HD11	3:C:99:VAL:H	1.56	0.71
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.06	0.71
10:J:19:SER:HA	10:J:22:LYS:NZ	2.05	0.71
19:S:5:LEU:O	19:S:6:LYS:HB2	1.90	0.71
1:A:1196:U:OP1	1:A:1197:G:H5'	1.90	0.70
1:A:1499:A:O2'	1:A:1500:A:H5'	1.90	0.70
2:B:55:PHE:HD2	2:B:58:ILE:HD12	1.55	0.70
3:C:191:THR:HG21	3:C:193:TYR:CZ	2.26	0.70
11:K:54:ARG:HH11	11:K:54:ARG:HB3	1.54	0.70
1:A:617:G:H5'	16:P:45:THR:HG22	1.73	0.70
1:A:1321:C:H42	19:S:37:ARG:HH12	1.39	0.70
9:I:51:ARG:HG2	9:I:56:LEU:HD12	1.73	0.70
10:J:81:THR:HG22	10:J:85:LEU:HD12	1.72	0.70
1:A:953:G:H1'	13:M:125:ARG:HA	1.72	0.70
1:A:959:A:H3'	1:A:960:U:H5"	1.73	0.70
2:B:178:ARG:NH1	2:B:178:ARG:HG3	2.02	0.70
1:A:579:G:H5'	1:A:728:A:H1'	1.74	0.70
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.55	0.70
21:U:9:ARG:NH1	21:U:23:PRO:HD2	2.02	0.70
1:A:266:G:C8	1:A:266:G:H5'	2.27	0.70
3:C:58:GLU:HB2	3:C:65:ALA:HB2	1.72	0.70
12:L:40:VAL:O	12:L:40:VAL:HG12	1.91	0.70
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.73	0.70
8:H:120:THR:OG1	8:H:123:GLU:HG3	1.90	0.70
10:J:9:ARG:HB3	10:J:9:ARG:NH1	2.06	0.70
1:A:81:U:C6	1:A:81:U:H5'	2.25	0.70
2:B:116:GLU:HG2	2:B:153:ARG:HH22	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:G:O2'	1:A:819:A:H5"	1.92	0.70
21:U:9:ARG:NH1	21:U:22:ARG:HA	2.06	0.70
1:A:1351:U:O2'	1:A:1352:C:H5'	1.91	0.69
2:B:76:GLN:NE2	2:B:207:ALA:H	1.89	0.69
17:Q:53:LEU:N	17:Q:53:LEU:HD12	2.04	0.69
5:E:144:THR:O	5:E:148:VAL:HG23	1.92	0.69
8:H:103:VAL:HG21	8:H:109:ILE:O	1.92	0.69
7:G:54:THR:HG22	7:G:55:GLY:N	2.07	0.69
13:M:11:ARG:HG3	13:M:12:ASN:N	2.07	0.69
6:F:101:ALA:HA	18:R:28:GLU:HG3	1.71	0.69
1:A:1502:A:H2	1:A:1505:G:N1	1.91	0.69
1:A:1392:G:H21	1:A:1502:A:H8	1.38	0.69
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.73	0.69
9:I:111:ARG:HD2	9:I:113:LYS:HD2	1.73	0.69
15:O:36:ILE:O	15:O:40:SER:HB2	1.92	0.69
1:A:130:A:C8	17:Q:63:ARG:HG3	2.27	0.69
5:E:18:ARG:HH21	5:E:25:ARG:HB3	1.58	0.69
10:J:84:GLN:O	10:J:88:LEU:HD12	1.93	0.69
12:L:55:VAL:HG12	12:L:56:ALA:N	2.06	0.69
1:A:1182:G:O2'	1:A:1183:A:OP2	2.09	0.69
2:B:19:HIS:NE2	2:B:206:ASP:HB3	2.07	0.69
16:P:74:LEU:O	16:P:79:VAL:HG23	1.93	0.69
5:E:101:ILE:HD12	5:E:119:LEU:HD23	1.75	0.69
16:P:34:GLU:OE2	16:P:55:ARG:HD3	1.92	0.69
1:A:1305:G:N2	1:A:1331:G:O2'	2.25	0.69
4:D:127:THR:CG2	4:D:147:ALA:HB3	2.22	0.69
19:S:17:GLU:HA	19:S:20:LEU:CG	2.22	0.69
22:X:39:A:O2'	22:X:40:U:H5'	1.92	0.69
2:B:12:GLU:OE2	2:B:213:LEU:HD11	1.92	0.69
2:B:84:GLU:HB3	2:B:219:VAL:CG2	2.18	0.69
1:A:1311:G:N7	19:S:2:PRO:HA	2.08	0.69
1:A:1281:U:H5'	1:A:1282:C:C5	2.27	0.69
1:A:130:A:OP2	1:A:190(E):U:H2'	1.92	0.69
1:A:344:A:H4'	1:A:345:C:OP2	1.92	0.69
1:A:673:G:H2'	1:A:674:G:C8	2.28	0.69
2:B:118:LEU:HB3	2:B:142:LEU:HD11	1.75	0.69
18:R:19:LYS:HD2	18:R:20:ALA:N	2.08	0.68
1:A:1256:A:O3'	1:A:1257:U:H4'	1.93	0.68
12:L:75:HIS:CD2	12:L:77:LEU:H	2.10	0.68
19:S:52:TYR:HA	19:S:56:GLN:O	1.93	0.68
1:A:1145:C:O2'	1:A:1146:A:H8	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:48:GLU:N	9:I:49:PRO:HD2	2.07	0.68
3:C:86:VAL:O	3:C:89:GLU:HB3	1.93	0.68
1:A:414:A:H2'	1:A:416:G:H22	1.58	0.68
1:A:1112:C:O2	3:C:179:ARG:HB3	1.92	0.68
1:A:1320:C:H41	19:S:37:ARG:NH1	1.90	0.68
2:B:137:ARG:HA	2:B:140:HIS:HD2	1.59	0.68
17:Q:59:ILE:HG22	17:Q:71:PHE:CD1	2.28	0.68
18:R:37:VAL:O	18:R:41:LYS:HG3	1.93	0.68
20:T:67:ALA:HA	20:T:73:HIS:H	1.59	0.68
4:D:119:GLN:HG2	4:D:123:HIS:CD2	2.28	0.68
4:D:151:LYS:H	4:D:151:LYS:CD	1.91	0.68
12:L:93:LEU:HB2	12:L:96:VAL:CG2	2.24	0.68
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.74	0.68
1:A:1367:C:H5'	10:J:60:ARG:HH12	1.57	0.68
12:L:27:LEU:O	12:L:29:GLY:N	2.27	0.68
12:L:47:LYS:CB	12:L:48:PRO:CD	2.67	0.68
13:M:50:GLU:O	13:M:54:VAL:HG23	1.93	0.68
1:A:1072:G:H2'	1:A:1073:U:C6	2.29	0.68
1:A:1178:G:N2	1:A:1180:A:H3'	2.09	0.68
1:A:328:C:O2	1:A:328:C:C2'	2.41	0.68
2:B:86:GLU:C	2:B:88:ALA:H	1.97	0.68
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.75	0.68
1:A:80:G:H2'	1:A:81:U:H5"	1.76	0.68
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.75	0.68
1:A:524:G:H2'	1:A:525:C:C6	2.30	0.67
8:H:83:ILE:O	8:H:83:ILE:HG23	1.94	0.67
1:A:1305:G:H5"	21:U:4:GLY:C	2.15	0.67
1:A:393:A:O2'	1:A:394:G:H5'	1.95	0.67
13:M:23:TYR:O	13:M:25:ILE:N	2.26	0.67
1:A:1064:G:H4'	1:A:1065:U:C5'	2.24	0.67
2:B:103:THR:HG23	2:B:176:GLU:OE1	1.94	0.67
3:C:91:LEU:HD11	3:C:99:VAL:HG22	1.75	0.67
6:F:1:MET:HB3	6:F:68:PRO:HA	1.76	0.67
10:J:26:ALA:C	10:J:84:GLN:HE21	1.98	0.67
19:S:12:ASP:H	19:S:38:SER:HB3	1.59	0.67
2:B:161:ALA:HB1	2:B:185:ILE:CD1	2.24	0.67
1:A:1231:G:H4'	9:I:126:SER:CB	2.25	0.67
22:X:35:C:H2'	22:X:36:G:H8	1.59	0.67
1:A:1392:G:N2	1:A:1502:A:H8	1.92	0.67
8:H:38:ILE:H	8:H:38:ILE:HD12	1.57	0.67
2:B:218:ALA:O	2:B:222:ILE:HG13	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:162:LEU:HD13	4:D:181:MET:HG2	1.76	0.67
6:F:26:ILE:O	6:F:30:LEU:HG	1.94	0.67
13:M:81:LEU:O	13:M:86:CYS:HB3	1.94	0.67
15:O:88:ARG:HB2	15:O:88:ARG:HH11	1.56	0.67
4:D:146:ILE:HD12	4:D:146:ILE:N	2.09	0.67
22:X:35:C:H42	23:Y:3:G:H1	1.43	0.67
7:G:18:TYR:HD2	7:G:59:LEU:HD22	1.60	0.67
1:A:701:C:H5'	1:A:703:G:O4'	1.95	0.67
10:J:12:ASP:HB3	10:J:15:THR:HB	1.77	0.67
10:J:30:SER:OG	10:J:81:THR:HA	1.94	0.67
12:L:126:LYS:N	12:L:126:LYS:HE3	2.09	0.67
14:N:21:TYR:HE2	14:N:23:ARG:NE	1.93	0.67
13:M:52:GLU:HG2	13:M:55:ARG:HH21	1.60	0.67
13:M:6:GLY:O	13:M:7:VAL:HG22	1.95	0.67
1:A:444:C:H6	1:A:491:G:H22	1.42	0.66
6:F:33:TYR:HA	6:F:71:ARG:NH2	2.00	0.66
7:G:116:ALA:HA	7:G:119:ARG:NH2	2.10	0.66
7:G:92:SER:HB2	7:G:93:PRO:HD2	1.77	0.66
1:A:417:C:H3'	1:A:418:C:C6	2.29	0.66
1:A:55:A:O2'	1:A:56:U:H5'	1.96	0.66
4:D:111:ALA:HA	4:D:161:ASN:ND2	2.10	0.66
12:L:27:LEU:C	12:L:29:GLY:H	1.99	0.66
6:F:47:ARG:HE	6:F:47:ARG:N	1.90	0.66
10:J:59:SER:O	10:J:60:ARG:HB2	1.94	0.66
12:L:27:LEU:HG	12:L:28:LYS:H	1.60	0.66
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.76	0.66
1:A:1103:C:C5'	2:B:98:LEU:HD12	2.26	0.66
5:E:129:ILE:HD12	5:E:129:ILE:H	1.59	0.66
7:G:70:LYS:HB3	7:G:96:GLN:HG2	1.77	0.66
1:A:706:A:O4'	11:K:29:ILE:HD11	1.96	0.66
1:A:409:G:H1	1:A:434:U:H5	1.43	0.66
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.06	0.66
1:A:1151:A:HO2'	1:A:1152:A:H8	1.43	0.66
6:F:101:ALA:CB	18:R:28:GLU:HG3	2.25	0.66
1:A:168:G:O2'	1:A:169:C:H5'	1.96	0.66
1:A:337:C:H2'	1:A:338:A:H8	1.61	0.66
2:B:25:ASN:C	2:B:25:ASN:HD22	1.99	0.66
3:C:25:GLY:O	3:C:27:LYS:N	2.25	0.66
3:C:70:VAL:HG12	3:C:71:ALA:N	2.11	0.66
4:D:18:LYS:NZ	4:D:33:MET:HB2	2.11	0.66
4:D:3:ARG:HG3	4:D:118:ARG:CZ	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:C:H1'	8:H:3:THR:CG2	2.26	0.66
1:A:279:A:H5"	1:A:280:C:H3'	1.77	0.66
5:E:8:GLU:HG2	5:E:34:VAL:HG22	1.78	0.66
1:A:835:U:OP1	18:R:64:ARG:NH2	2.29	0.66
19:S:3:ARG:HH22	19:S:69:HIS:CE1	2.13	0.66
1:A:882:C:O2'	1:A:883:C:H5'	1.95	0.66
3:C:108:ASN:ND2	3:C:111:LEU:HG	2.08	0.66
15:O:82:ILE:HD13	15:O:88:ARG:HH22	1.60	0.66
8:H:90:GLY:O	8:H:91:ARG:HB2	1.95	0.66
12:L:89:ARG:CZ	12:L:97:ARG:HE	2.09	0.66
4:D:25:ARG:C	4:D:27:TYR:H	1.99	0.65
7:G:139:GLU:O	7:G:143:ARG:HG3	1.97	0.65
1:A:1121:U:H2'	1:A:1122:U:C6	2.31	0.65
10:J:32:ALA:HB2	10:J:76:ASN:HD22	1.60	0.65
1:A:1391:U:H2'	1:A:1392:G:H8	1.62	0.65
12:L:83:VAL:HG13	12:L:100:ILE:HG23	1.78	0.65
1:A:839:U:O2	1:A:839:U:H2'	1.96	0.65
3:C:21:ARG:HH22	3:C:56:ASP:HB3	1.60	0.65
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.78	0.65
12:L:86:ARG:HG3	12:L:86:ARG:HH11	1.61	0.65
13:M:33:ALA:HA	13:M:59:TYR:CE2	2.32	0.65
20:T:10:LEU:O	20:T:13:LEU:HG	1.97	0.65
1:A:1040:U:H2'	1:A:1041:A:C8	2.31	0.65
1:A:1223:C:P	19:S:78:ARG:HH12	2.19	0.65
5:E:151:LEU:HD22	8:H:79:VAL:HA	1.77	0.65
20:T:50:GLU:N	20:T:99:LEU:HD12	2.09	0.65
10:J:3:LYS:N	10:J:75:ILE:HA	2.11	0.65
1:A:1125:U:H3	10:J:5:ARG:NH2	1.93	0.65
6:F:1:MET:HB2	6:F:67:MET:O	1.96	0.65
1:A:1397:C:H4'	1:A:1398:A:OP2	1.96	0.65
2:B:136:VAL:HG12	2:B:140:HIS:NE2	2.12	0.65
3:C:118:GLN:O	3:C:122:GLU:HG3	1.96	0.65
3:C:119:ARG:HG2	3:C:140:ARG:NH1	2.12	0.65
10:J:16:LEU:HD13	10:J:70:ARG:HG2	1.78	0.65
1:A:1427:U:H2'	1:A:1428:A:C8	2.32	0.65
1:A:327:A:O2'	1:A:328:C:O4'	2.15	0.65
9:I:24:GLY:HA2	9:I:59:PHE:O	1.96	0.65
13:M:10:PRO:CB	13:M:18:ALA:HB1	2.21	0.65
3:C:156:ARG:HH21	3:C:161:GLU:HA	1.62	0.65
3:C:6:HIS:HD2	3:C:8:ILE:H	1.43	0.65
4:D:78:LEU:HD22	4:D:96:LEU:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:8:LEU:CD1	10:J:20:ALA:HB2	2.26	0.65
2:B:111:ARG:HB3	2:B:149:LEU:HD11	1.77	0.64
2:B:18:GLY:CA	2:B:41:ILE:HA	2.26	0.64
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.78	0.64
1:A:1298:C:H4'	1:A:1299:A:O4'	1.97	0.64
1:A:946:A:H2'	1:A:947:G:C8	2.32	0.64
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.79	0.64
12:L:59:ARG:HH21	12:L:65:GLU:HB3	1.61	0.64
1:A:1481:U:O2'	1:A:1482:G:H5'	1.97	0.64
1:A:5:U:H4'	1:A:6:G:O5'	1.96	0.64
2:B:219:VAL:HA	2:B:222:ILE:HD12	1.80	0.64
2:B:82:ARG:O	2:B:86:GLU:HG3	1.97	0.64
13:M:125:ARG:HD2	13:M:125:ARG:C	2.18	0.64
1:A:1263:C:H2'	1:A:1264:C:C6	2.32	0.64
1:A:1497:G:C2'	1:A:1498:U:H5'	2.28	0.64
2:B:132:LYS:HA	2:B:135:GLN:OE1	1.97	0.64
3:C:84:ILE:HG12	3:C:88:ARG:HH11	1.63	0.64
5:E:15:ARG:HD3	5:E:26:PHE:CD2	2.33	0.64
2:B:140:HIS:O	2:B:143:GLU:HB2	1.98	0.64
2:B:166:ASP:OD2	2:B:169:LYS:HB2	1.98	0.64
19:S:80:TYR:CE2	19:S:81:ARG:HB3	2.33	0.64
22:X:35:C:H2'	22:X:36:G:C8	2.33	0.64
7:G:111:ARG:HB3	7:G:113:GLU:OE2	1.98	0.64
1:A:1130:A:OP2	1:A:1130:A:H3'	1.98	0.64
2:B:178:ARG:NH2	8:H:68:ARG:HH22	1.95	0.64
10:J:16:LEU:HD23	10:J:94:VAL:HG22	1.79	0.64
13:M:65:LYS:HG3	13:M:69:GLU:OE2	1.97	0.64
1:A:1241:G:H2'	1:A:1242:C:C6	2.33	0.64
1:A:1277:C:C2'	1:A:1278:U:H5'	2.28	0.64
1:A:414:A:H2'	1:A:416:G:N1	2.13	0.64
1:A:818:G:C3'	1:A:819:A:H5"	2.27	0.64
3:C:191:THR:CG2	3:C:192:THR:N	2.60	0.64
7:G:72:ARG:O	7:G:73:MET:HG2	1.97	0.64
18:R:19:LYS:HZ3	18:R:55:ARG:HH11	1.45	0.64
19:S:40:ILE:HG21	19:S:62:ILE:HD13	1.79	0.64
1:A:1223:C:OP1	1:A:1224:G:H3'	1.98	0.63
1:A:1287:A:H2'	1:A:1288:A:C8	2.32	0.63
3:C:119:ARG:HG2	3:C:140:ARG:HH12	1.62	0.63
5:E:18:ARG:NH2	5:E:25:ARG:HB3	2.14	0.63
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.33	0.63
1:A:1412:C:H2'	1:A:1413:A:C8	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:G:H2'	1:A:792:A:C5'	2.28	0.63
6:F:100:ASN:CA	18:R:23:LYS:HE3	2.28	0.63
1:A:1040:U:H2'	1:A:1041:A:H8	1.63	0.63
1:A:1141:C:H2'	1:A:1142:G:H8	1.63	0.63
1:A:1218:C:H2'	1:A:1219:U:C6	2.33	0.63
1:A:35:G:H2'	1:A:36:C:H6	1.64	0.63
2:B:23:ARG:HD3	2:B:24:TRP:N	2.13	0.63
4:D:57:ARG:HG3	4:D:57:ARG:HH11	1.62	0.63
4:D:62:GLN:HA	4:D:62:GLN:NE2	2.13	0.63
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.81	0.63
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.62	0.63
13:M:78:ILE:HA	13:M:81:LEU:HD21	1.80	0.63
13:M:3:ARG:HA	13:M:8:GLU:O	1.99	0.63
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.33	0.63
3:C:116:VAL:HG11	3:C:141:VAL:HG21	1.81	0.63
3:C:131:ARG:O	3:C:135:LYS:HG3	1.99	0.63
5:E:57:LYS:HG2	5:E:61:TYR:CE2	2.33	0.63
10:J:4:ILE:O	10:J:73:ASP:HA	1.99	0.63
13:M:77:ASN:O	13:M:81:LEU:HD22	1.99	0.63
1:A:1477:C:H2'	1:A:1478:C:H6	1.64	0.63
1:A:662:G:H2'	1:A:663:A:C8	2.33	0.63
9:I:106:ALA:O	9:I:108:VAL:HG23	1.99	0.63
7:G:50:ILE:HA	7:G:125:MET:HE2	1.81	0.63
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.81	0.63
1:A:1247:U:O2'	1:A:1248:A:H5'	1.98	0.63
1:A:1435:G:H2'	1:A:1436:U:C6	2.33	0.63
1:A:337:C:H2'	1:A:338:A:C8	2.34	0.63
1:A:437:U:O2'	1:A:438:G:H5'	1.97	0.63
3:C:79:ARG:HG3	3:C:79:ARG:O	1.99	0.63
1:A:818:G:C2'	1:A:819:A:H5"	2.29	0.62
2:B:231:GLU:CD	2:B:231:GLU:H	2.02	0.62
7:G:78:ARG:HD2	7:G:156:TRP:HZ3	1.64	0.62
3:C:83:ARG:C	3:C:85:ARG:H	2.02	0.62
12:L:24:VAL:HG12	12:L:24:VAL:O	1.99	0.62
4:D:18:LYS:HZ3	4:D:33:MET:HB2	1.63	0.62
1:A:166:G:O2'	1:A:167:G:H5'	1.98	0.62
13:M:105:THR:O	13:M:106:ASN:HB2	1.97	0.62
19:S:17:GLU:O	19:S:21:GLU:HG3	2.00	0.62
13:M:3:ARG:NH2	13:M:7:VAL:HG12	2.14	0.62
1:A:1042:G:O2'	1:A:1043:C:H5'	1.99	0.62
1:A:1347:G:H22	1:A:1373:G:H2'	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:C:O2'	1:A:813:U:P	2.57	0.62
1:A:973:G:H3'	1:A:974:A:H5"	1.81	0.62
6:F:46:ARG:HE	6:F:47:ARG:NH2	1.98	0.62
11:K:84:VAL:HG11	11:K:95:ILE:HD11	1.80	0.62
1:A:1116:C:H2'	1:A:1117:G:C5'	2.30	0.62
1:A:353:A:H5'	1:A:353:A:H8	1.64	0.62
2:B:118:LEU:HD13	2:B:142:LEU:HG	1.81	0.62
2:B:91:PRO:HG2	2:B:155:LEU:HD23	1.80	0.62
3:C:77:ILE:O	3:C:83:ARG:HB3	1.99	0.62
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.82	0.62
2:B:178:ARG:HH21	8:H:68:ARG:HH22	1.45	0.62
13:M:79:LYS:HG2	13:M:83:ASP:OD2	2.00	0.62
18:R:43:PHE:HA	18:R:51:LEU:HD12	1.80	0.62
1:A:412:A:C1'	1:A:413:G:H2'	2.29	0.62
1:A:448:A:H2'	1:A:449:C:C6	2.35	0.62
1:A:556:C:O2'	1:A:557:G:H5'	1.99	0.62
1:A:627:G:O2'	1:A:628:G:H5'	2.00	0.62
3:C:89:GLU:HG3	3:C:93:LYS:HE2	1.82	0.62
9:I:32:ASP:O	9:I:35:GLU:HB3	2.00	0.62
10:J:90:LEU:N	10:J:91:PRO:HD2	2.10	0.62
11:K:69:ALA:O	11:K:73:MET:HG2	1.99	0.62
12:L:24:VAL:O	12:L:26:ALA:N	2.29	0.62
1:A:1176:A:H2'	1:A:1177:G:C8	2.35	0.61
1:A:67:C:O2'	1:A:171:A:H1'	2.00	0.61
1:A:975:A:H4'	1:A:976:G:O5'	2.00	0.61
2:B:204:ASN:HD22	2:B:210:SER:HB2	1.65	0.61
10:J:94:VAL:HG12	10:J:95:GLU:N	2.14	0.61
21:U:5:ASP:O	21:U:11:GLY:HA3	2.00	0.61
1:A:1161:C:H2'	1:A:1162:C:H6	1.65	0.61
1:A:1477:C:H2'	1:A:1478:C:C6	2.35	0.61
1:A:371:G:C2'	1:A:372:C:H5'	2.29	0.61
1:A:620:C:N1	4:D:135:LEU:HD13	2.15	0.61
1:A:437:U:H5"	4:D:155:LEU:HD22	1.81	0.61
1:A:975:A:H5'	1:A:975:A:C8	2.35	0.61
3:C:39:ILE:HD12	3:C:57:ILE:HD13	1.82	0.61
19:S:29:ARG:N	19:S:29:ARG:HD2	2.16	0.61
1:A:1004:A:H5"	1:A:1025:U:C4	2.35	0.61
3:C:127:ARG:HH11	3:C:127:ARG:HG3	1.65	0.61
12:L:27:LEU:C	12:L:29:GLY:N	2.53	0.61
6:F:100:ASN:CB	18:R:23:LYS:HE3	2.30	0.61
1:A:1504:G:H3'	1:A:1504:G:OP2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:2001:PAR:HN61	24:A:2001:PAR:H34	1.65	0.61
1:A:580:U:H2'	1:A:581:G:O4'	2.01	0.61
11:K:126:ARG:O	11:K:127:LYS:HB2	2.00	0.61
3:C:191:THR:HG21	3:C:193:TYR:CE1	2.35	0.61
15:O:22:THR:O	15:O:27:VAL:HG11	2.00	0.61
1:A:242:C:H2'	1:A:243:A:H5'	1.81	0.61
6:F:2:ARG:CD	6:F:69:GLU:HG2	2.31	0.61
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.83	0.61
11:K:57:THR:HG23	11:K:60:ALA:H	1.66	0.61
1:A:539:A:H2'	1:A:540:G:C8	2.35	0.61
12:L:85:ILE:HG23	12:L:98:TYR:HB3	1.83	0.61
14:N:9:LYS:HD3	14:N:9:LYS:C	2.21	0.61
1:A:1343:G:H2'	1:A:1344:C:C6	2.36	0.61
2:B:9:GLU:C	2:B:10:LEU:HD12	2.21	0.61
17:Q:60:ILE:HB	17:Q:74:LEU:HB2	1.82	0.61
20:T:50:GLU:HA	20:T:100:ILE:HG22	1.83	0.61
2:B:69:LEU:HD23	2:B:70:PHE:N	2.15	0.61
5:E:103:GLY:O	5:E:106:PRO:HD2	2.01	0.60
16:P:17:TYR:HE1	16:P:41:PRO:HG2	1.66	0.60
1:A:1096:C:H2'	1:A:1097:C:H6	1.66	0.60
1:A:1216:G:H5"	14:N:5:ALA:CB	2.32	0.60
3:C:102:ASN:N	3:C:102:ASN:HD22	1.97	0.60
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.82	0.60
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.83	0.60
6:F:53:ALA:C	6:F:55:ASP:H	2.03	0.60
7:G:15:ASP:O	7:G:19:GLY:HA2	2.01	0.60
19:S:62:ILE:HD12	19:S:66:MET:HG3	1.83	0.60
20:T:53:LEU:HB2	20:T:100:ILE:CG2	2.32	0.60
1:A:1118:C:H1'	1:A:1179:A:C4	2.36	0.60
1:A:444:C:H2'	1:A:491:G:H22	1.66	0.60
1:A:853:G:O2'	1:A:854:G:H5'	2.00	0.60
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.81	0.60
6:F:68:PRO:HB2	6:F:71:ARG:HG3	1.82	0.60
10:J:34:VAL:CA	10:J:75:ILE:HG22	2.30	0.60
12:L:83:VAL:HG11	12:L:100:ILE:HD13	1.83	0.60
12:L:57:LYS:HD3	12:L:67:THR:HG22	1.82	0.60
3:C:70:VAL:O	3:C:106:VAL:HG23	2.02	0.60
5:E:120:THR:HG23	5:E:121:LYS:N	2.15	0.60
1:A:932:C:H5'	7:G:4:ARG:HG2	1.83	0.60
10:J:27:ALA:HB2	10:J:85:LEU:HD11	1.83	0.60
1:A:190(L):U:O2	20:T:105:SER:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1544:U:H4'	23:Y:1:U:OP2	2.01	0.60
1:A:1064:G:H4'	1:A:1065:U:H5'	1.82	0.60
1:A:1117:G:H5'	1:A:1117:G:H8	1.65	0.60
6:F:101:ALA:CA	18:R:28:GLU:HG3	2.32	0.60
1:A:1152:A:H5"	10:J:13:HIS:HB2	1.82	0.60
1:A:1238:A:H5'	1:A:1336:C:N4	2.12	0.60
1:A:352:C:H4'	1:A:354:G:OP1	1.99	0.60
2:B:137:ARG:HH11	2:B:137:ARG:HB3	1.66	0.60
2:B:139:LYS:O	2:B:139:LYS:HD3	2.01	0.60
19:S:63:THR:HG22	19:S:64:GLU:N	2.17	0.60
1:A:112:G:N2	1:A:354:G:H5'	2.12	0.60
7:G:75:VAL:CG2	7:G:86:GLN:HB3	2.31	0.60
18:R:25:THR:O	18:R:26:LEU:HB2	1.99	0.60
19:S:29:ARG:H	19:S:29:ARG:HD2	1.65	0.60
1:A:1305:G:H22	1:A:1331:G:C2'	2.15	0.60
1:A:1453:G:H2'	1:A:1454:G:O4'	2.02	0.60
1:A:190:C:H2'	1:A:190(A):C:C6	2.36	0.60
1:A:243:A:H4'	1:A:244:U:C5'	2.24	0.60
7:G:15:ASP:OD1	7:G:17:VAL:N	2.35	0.60
7:G:72:ARG:HA	7:G:96:GLN:NE2	2.15	0.60
10:J:90:LEU:N	10:J:91:PRO:CD	2.64	0.60
1:A:794:A:H2'	1:A:795:C:C6	2.36	0.60
3:C:58:GLU:HB2	3:C:65:ALA:CB	2.32	0.60
6:F:2:ARG:CZ	6:F:69:GLU:HG2	2.31	0.60
1:A:598:U:H4'	8:H:94:TYR:CD1	2.36	0.60
19:S:43:GLU:H	19:S:43:GLU:CD	2.05	0.60
20:T:56:MET:HE3	20:T:88:VAL:HG11	1.84	0.60
2:B:142:LEU:HB3	2:B:146:GLN:NE2	2.17	0.60
2:B:47:THR:HA	2:B:202:PRO:HG2	1.83	0.60
3:C:130:VAL:O	3:C:134:ILE:HG13	2.01	0.60
12:L:26:ALA:O	12:L:27:LEU:O	2.20	0.59
1:A:1216:G:H5"	14:N:5:ALA:HB2	1.85	0.59
6:F:1:MET:SD	6:F:66:GLU:HG2	2.43	0.59
1:A:877:C:H1'	8:H:3:THR:HG21	1.85	0.59
15:O:17:ARG:HH11	15:O:17:ARG:CG	2.09	0.59
1:A:127:G:HO2'	17:Q:2:PRO:N	1.99	0.59
19:S:37:ARG:O	19:S:70:LYS:HD2	2.02	0.59
1:A:1298:C:H2'	7:G:114:ARG:NH1	2.17	0.59
10:J:31:GLY:HA3	10:J:78:ASN:ND2	2.17	0.59
10:J:7:LYS:HE3	10:J:40:LEU:HD11	1.84	0.59
13:M:9:ILE:N	13:M:9:ILE:HD12	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:95:TYR:O	17:Q:97:SER:N	2.35	0.59
4:D:152:SER:O	4:D:158:ILE:HD12	2.02	0.59
6:F:47:ARG:O	6:F:47:ARG:HG2	2.02	0.59
12:L:25:PRO:C	12:L:27:LEU:H	2.04	0.59
1:A:101:A:O2'	1:A:102:G:H5'	2.02	0.59
1:A:1392:G:O2'	1:A:1502:A:H5"	2.01	0.59
2:B:53:ARG:HH12	2:B:199:TYR:HA	1.67	0.59
10:J:22:LYS:HE2	10:J:90:LEU:N	2.17	0.59
20:T:94:ALA:O	20:T:95:ALA:HB3	2.02	0.59
1:A:1288:A:H2'	1:A:1289:A:C8	2.37	0.59
3:C:10:PHE:CZ	3:C:178:LEU:HD13	2.38	0.59
4:D:156:GLU:HG2	4:D:160:GLN:HE21	1.67	0.59
1:A:254:G:OP1	17:Q:67:LYS:O	2.20	0.59
1:A:52:G:O2'	1:A:53:A:H5'	2.02	0.59
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.85	0.59
8:H:36:LEU:HD12	8:H:59:LEU:HD13	1.84	0.59
10:J:98:ILE:O	10:J:99:LYS:HD2	2.02	0.59
17:Q:98:LEU:HD23	17:Q:98:LEU:H	1.67	0.59
2:B:52:GLU:HG2	2:B:56:ARG:HH21	1.68	0.59
3:C:3:ASN:ND2	3:C:3:ASN:H	1.89	0.59
3:C:70:VAL:HG12	3:C:72:LYS:H	1.68	0.59
17:Q:53:LEU:H	17:Q:53:LEU:CD1	2.08	0.59
20:T:13:LEU:HD12	20:T:13:LEU:H	1.66	0.59
1:A:1003(A):G:H2'	1:A:1004:A:C4'	2.33	0.59
1:A:1470:G:O2'	1:A:1471:G:H5'	2.03	0.59
2:B:12:GLU:C	2:B:14:GLY:H	2.06	0.59
2:B:50:GLU:HB3	2:B:200:ILE:O	2.02	0.59
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.84	0.59
11:K:93:GLN:HE21	11:K:96:ARG:HH21	1.48	0.59
19:S:15:LEU:O	19:S:19:VAL:HG12	2.02	0.59
1:A:1004:A:H5"	1:A:1025:U:C5	2.38	0.59
1:A:1193:G:O2'	1:A:1194:U:H5'	2.03	0.59
1:A:1230:C:O2'	1:A:1231:G:H5'	2.03	0.59
1:A:390:C:H2'	1:A:391:G:C8	2.38	0.59
1:A:417:C:H2'	1:A:418:C:O4'	2.03	0.59
1:A:791:G:H2'	1:A:792:A:H5'	1.85	0.59
1:A:807:A:H2'	1:A:808:C:C6	2.38	0.59
15:O:71:GLN:O	15:O:71:GLN:HG2	2.02	0.59
16:P:45:THR:HB	16:P:46:PRO:HD2	1.84	0.59
1:A:1106:G:H5"	3:C:172:ARG:HG2	1.83	0.58
2:B:36:ARG:HD2	2:B:41:ILE:CD1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:GLY:HA3	2:B:81:VAL:HG21	1.84	0.58
12:L:93:LEU:HB2	12:L:96:VAL:HG21	1.85	0.58
13:M:82:MET:CE	13:M:92:HIS:HB3	2.32	0.58
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.39	0.58
1:A:105:G:H2'	1:A:106:C:C6	2.38	0.58
1:A:19:C:H2'	1:A:20:U:H6	1.68	0.58
3:C:148:GLY:HA3	3:C:172:ARG:O	2.03	0.58
1:A:1152:A:H5"	10:J:13:HIS:HD2	1.66	0.58
6:F:80:ARG:NH1	6:F:88:VAL:O	2.37	0.58
12:L:45:PRO:HD3	12:L:51:ALA:O	2.03	0.58
13:M:17:VAL:O	13:M:20:THR:HB	2.03	0.58
15:O:87:ILE:HG22	15:O:88:ARG:NE	2.18	0.58
19:S:53:ASN:ND2	19:S:56:GLN:HB2	2.18	0.58
1:A:1352:C:H2'	1:A:1353:G:C8	2.38	0.58
1:A:406:G:H21	4:D:119:GLN:HE22	1.52	0.58
1:A:421:U:H5'	1:A:422:C:H5	1.67	0.58
1:A:639:G:O2'	1:A:640:A:H5'	2.03	0.58
10:J:7:LYS:HE3	10:J:40:LEU:CD1	2.32	0.58
1:A:523:A:H61	12:L:92:ASP:HB2	1.68	0.58
13:M:19:LEU:HD11	13:M:34:LEU:HD21	1.86	0.58
1:A:1128:C:O2'	1:A:1130:A:C8	2.56	0.58
1:A:1320:C:O2	19:S:72:GLY:HA3	2.04	0.58
1:A:269:C:H2'	1:A:270:A:C8	2.39	0.58
5:E:12:LEU:CD1	5:E:31:LEU:HB2	2.33	0.58
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.85	0.58
17:Q:69:LYS:C	17:Q:70:ARG:HD2	2.23	0.58
1:A:1532:U:C2'	1:A:1533:C:H4'	2.33	0.58
1:A:113:G:H1'	1:A:354:G:H5'	1.86	0.58
2:B:187:LEU:HA	2:B:201:ILE:HB	1.86	0.58
4:D:31:CYS:SG	4:D:31:CYS:O	2.61	0.58
18:R:19:LYS:HZ3	18:R:55:ARG:HD2	1.67	0.58
1:A:1305:G:H5'	21:U:4:GLY:HA3	1.86	0.58
1:A:1161:C:H2'	1:A:1162:C:C6	2.38	0.58
1:A:407:G:H2'	1:A:408:A:C8	2.38	0.58
1:A:490:G:O2'	1:A:491:G:H5'	2.03	0.58
1:A:998:G:O2'	1:A:999:C:H5'	2.02	0.58
7:G:115:ARG:HB2	7:G:118:VAL:CG2	2.33	0.58
9:I:43:ALA:N	9:I:74:ILE:HD13	2.18	0.58
15:O:70:LEU:HD12	15:O:78:TYR:CA	2.33	0.58
19:S:30:LEU:HA	19:S:48:THR:O	2.03	0.58
22:X:38:A:H2'	22:X:39:A:O4'	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:G:H5'	1:A:389:A:H4'	1.85	0.58
1:A:1424:C:O2'	1:A:1425:U:H5'	2.04	0.58
1:A:1533:C:O2	1:A:1533:C:H2'	2.03	0.58
1:A:1533:C:O2	1:A:1533:C:H5"	2.03	0.58
1:A:865:A:H5'	1:A:1078:U:O4	2.04	0.58
2:B:16:HIS:CE1	2:B:214:ILE:HD11	2.39	0.58
2:B:223:ILE:HD12	2:B:224:GLN:H	1.68	0.58
10:J:69:ASN:O	10:J:70:ARG:NE	2.37	0.58
11:K:72:ALA:O	11:K:77:MET:HB2	2.04	0.58
13:M:8:GLU:OE1	13:M:22:ILE:HA	2.04	0.58
1:A:203:U:H5"	1:A:204:U:OP1	2.04	0.58
1:A:384:G:H2'	1:A:385:C:C6	2.39	0.58
1:A:414:A:H8	1:A:416:G:N1	1.90	0.58
2:B:204:ASN:HD22	2:B:210:SER:CB	2.16	0.58
5:E:121:LYS:HD2	5:E:122:GLU:N	2.19	0.58
7:G:135:VAL:O	7:G:139:GLU:HG3	2.03	0.58
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.86	0.58
11:K:48:ILE:HG13	11:K:64:ALA:N	2.18	0.58
9:I:31:GLN:HB3	9:I:35:GLU:HG2	1.86	0.58
16:P:5:ARG:HH21	16:P:28:ARG:HA	1.69	0.58
1:A:1066:C:O2'	1:A:1067:A:H5'	2.04	0.57
1:A:21:G:H2'	1:A:22:G:C8	2.39	0.57
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.85	0.57
1:A:1539:C:N4	7:G:82:GLY:HA2	2.19	0.57
10:J:26:ALA:O	10:J:84:GLN:HG3	2.03	0.57
13:M:33:ALA:HA	13:M:59:TYR:HE2	1.68	0.57
17:Q:86:GLU:O	17:Q:90:ILE:HG13	2.04	0.57
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.39	0.57
1:A:1068:G:H8	1:A:1068:G:OP2	1.87	0.57
1:A:407:G:H2'	1:A:408:A:H8	1.69	0.57
15:O:6:GLU:CD	15:O:6:GLU:H	2.06	0.57
16:P:26:ARG:HD3	16:P:31:LYS:N	2.19	0.57
1:A:392:G:H2'	1:A:393:A:C8	2.39	0.57
1:A:1115:C:H1'	14:N:61:TRP:O	2.04	0.57
1:A:1132:C:H2'	1:A:1133:G:H8	1.69	0.57
1:A:178:C:O2'	1:A:179:A:H5'	2.04	0.57
2:B:142:LEU:HB3	2:B:146:GLN:HE21	1.69	0.57
20:T:29:LYS:O	20:T:33:ILE:HG13	2.04	0.57
1:A:1236:A:H4'	1:A:1304:G:H4'	1.86	0.57
1:A:411:A:H4'	1:A:429:U:O4	2.04	0.57
5:E:121:LYS:HD2	5:E:122:GLU:H	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:19:SER:HB2	10:J:91:PRO:HB3	1.86	0.57
11:K:14:VAL:HG21	11:K:40:ILE:HD11	1.86	0.57
14:N:26:ARG:HE	14:N:47:LEU:HD21	1.69	0.57
18:R:17:SER:HB2	18:R:54:ARG:HH21	1.68	0.57
19:S:20:LEU:HA	19:S:23:ASN:ND2	2.19	0.57
1:A:114:U:O2'	1:A:115:G:H5'	2.05	0.57
1:A:1250:A:H5'	9:I:68:GLY:O	2.04	0.57
1:A:961:U:C2'	1:A:962:C:H5'	2.33	0.57
2:B:116:GLU:HG2	2:B:153:ARG:NH2	2.20	0.57
3:C:156:ARG:NH2	3:C:161:GLU:HA	2.19	0.57
4:D:24:GLU:H	4:D:112:VAL:CG1	2.17	0.57
7:G:145:ALA:O	7:G:146:GLU:HB3	2.05	0.57
9:I:82:ALA:HB1	9:I:96:LEU:HD23	1.86	0.57
13:M:22:ILE:O	13:M:23:TYR:O	2.22	0.57
1:A:1025:U:H2'	1:A:1026:G:C8	2.40	0.57
1:A:1372:U:H2'	1:A:1373:G:O4'	2.04	0.57
1:A:1372:U:O2'	1:A:1373:G:H5'	2.05	0.57
1:A:448:A:OP2	1:A:485:G:N2	2.25	0.57
3:C:110:ASN:O	3:C:111:LEU:HD23	2.04	0.57
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.86	0.57
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.85	0.57
19:S:5:LEU:O	19:S:6:LYS:CB	2.52	0.57
1:A:664:G:OP1	18:R:64:ARG:HD2	2.04	0.57
6:F:91:VAL:HG11	18:R:72:ARG:NH1	2.20	0.57
1:A:433:C:H2'	1:A:434:U:N3	2.20	0.57
2:B:206:ASP:O	2:B:207:ALA:HB3	2.05	0.57
2:B:239:VAL:H	2:B:240:GLN:NE2	2.03	0.57
3:C:100:ALA:O	3:C:101:LEU:HB2	2.05	0.57
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.87	0.57
3:C:135:LYS:HE2	5:E:50:GLU:OE2	2.04	0.57
7:G:17:VAL:HG12	7:G:18:TYR:N	2.19	0.57
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.87	0.57
1:A:1003:G:N2	1:A:1039:C:C2	2.72	0.57
1:A:1106:G:OP1	3:C:172:ARG:HD3	2.04	0.57
1:A:1307:U:H2'	1:A:1308:U:C6	2.39	0.57
1:A:1522:U:O2'	1:A:1523:G:H5'	2.04	0.57
1:A:983:A:H5'	1:A:984:C:OP2	2.04	0.57
2:B:115:LEU:O	2:B:115:LEU:HD12	2.05	0.57
2:B:215:LEU:O	2:B:219:VAL:HG23	2.04	0.57
2:B:76:GLN:NE2	2:B:207:ALA:N	2.53	0.57
3:C:180:ALA:O	3:C:181:ASN:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:151:LYS:N	4:D:151:LYS:HD2	2.00	0.57
8:H:127:LEU:N	8:H:127:LEU:HD23	2.19	0.57
9:I:3:GLN:HG3	9:I:20:ARG:HG2	1.86	0.57
13:M:7:VAL:O	13:M:9:ILE:HG13	2.05	0.57
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.85	0.57
18:R:26:LEU:HD21	18:R:39:VAL:CG2	2.35	0.57
1:A:1014:A:H2'	1:A:1015:A:C8	2.40	0.56
1:A:1016:A:H2'	1:A:1017:G:O4'	2.04	0.56
5:E:57:LYS:HG2	5:E:61:TYR:HE2	1.67	0.56
7:G:156:TRP:CE3	7:G:156:TRP:HA	2.40	0.56
11:K:33:THR:HG22	11:K:39:PRO:HA	1.86	0.56
11:K:54:ARG:HH11	11:K:54:ARG:CB	2.17	0.56
10:J:49:VAL:CG1	14:N:41:ARG:HD2	2.34	0.56
17:Q:65:ILE:N	17:Q:65:ILE:HD12	2.19	0.56
1:A:994:A:N7	1:A:1216:G:H4'	2.20	0.56
1:A:1381:U:O2'	1:A:1382:C:H5'	2.05	0.56
1:A:1427:U:H2'	1:A:1428:A:H8	1.69	0.56
1:A:392:G:H2'	1:A:393:A:H8	1.69	0.56
1:A:421:U:H5'	1:A:422:C:C5	2.40	0.56
10:J:26:ALA:HB3	10:J:85:LEU:HD21	1.86	0.56
10:J:29:ARG:HB2	10:J:84:GLN:HE22	1.69	0.56
10:J:49:VAL:HG11	14:N:41:ARG:O	2.05	0.56
18:R:54:ARG:HD3	18:R:55:ARG:HG2	1.87	0.56
19:S:15:LEU:O	19:S:19:VAL:N	2.38	0.56
1:A:1355:G:O2'	1:A:1356:G:H5'	2.05	0.56
1:A:1497:G:H2'	1:A:1498:U:H5'	1.87	0.56
3:C:88:ARG:O	3:C:91:LEU:HB3	2.05	0.56
11:K:109:VAL:HG22	18:R:86:VAL:HG22	1.87	0.56
14:N:29:ARG:HB3	14:N:40:CYS:HB3	1.85	0.56
17:Q:4:LYS:HE3	17:Q:6:LEU:CD2	2.34	0.56
18:R:19:LYS:O	18:R:20:ALA:HB2	2.06	0.56
1:A:429:U:H1'	1:A:430:A:H5"	1.87	0.56
2:B:137:ARG:O	2:B:140:HIS:HB2	2.05	0.56
2:B:193:ASP:OD2	2:B:196:LEU:HG	2.05	0.56
2:B:239:VAL:H	2:B:240:GLN:HE22	1.50	0.56
3:C:14:ILE:O	3:C:16:ARG:N	2.38	0.56
8:H:6:ILE:O	8:H:10:LEU:HG	2.04	0.56
11:K:34:ASP:O	11:K:36:ASP:N	2.38	0.56
14:N:12:ARG:O	14:N:14:PRO:HD3	2.06	0.56
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.52	0.56
19:S:33:THR:HG22	19:S:34:TRP:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1305:G:C5'	21:U:4:GLY:HA3	2.35	0.56
1:A:80:G:C2'	1:A:81:U:H5"	2.35	0.56
1:A:818:G:H3'	1:A:819:A:C5'	2.36	0.56
1:A:912:C:O2'	1:A:913:A:H5'	2.05	0.56
1:A:960:U:O2	1:A:960:U:H5'	2.05	0.56
2:B:137:ARG:HA	2:B:140:HIS:CD2	2.41	0.56
6:F:36:ARG:HH21	6:F:38:GLU:HG2	1.71	0.56
7:G:45:ASP:O	7:G:49:ILE:HG13	2.06	0.56
13:M:37:THR:HG22	13:M:39:ILE:HG13	1.88	0.56
1:A:1320:C:N3	19:S:36:ARG:NH1	2.53	0.56
1:A:1356:G:H2'	1:A:1357:A:C8	2.41	0.56
1:A:269:C:H2'	1:A:270:A:H8	1.69	0.56
1:A:600:C:O2'	1:A:601:C:H5'	2.06	0.56
2:B:10:LEU:HG	2:B:48:MET:CE	2.35	0.56
2:B:167:PRO:HG3	2:B:188:ALA:HB2	1.88	0.56
2:B:18:GLY:HA2	2:B:40:HIS:O	2.06	0.56
2:B:76:GLN:HG3	2:B:206:ASP:OD1	2.05	0.56
10:J:14:LYS:HA	10:J:17:ASP:HB2	1.86	0.56
10:J:22:LYS:HE2	10:J:91:PRO:HD3	1.87	0.56
1:A:757:U:H2'	1:A:758:G:O4'	2.05	0.56
3:C:70:VAL:O	3:C:105:GLU:HA	2.05	0.56
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.85	0.56
4:D:187:ARG:CD	4:D:188:LEU:H	2.18	0.56
9:I:111:ARG:HD3	9:I:112:LYS:N	2.20	0.56
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.38	0.56
12:L:93:LEU:HB2	12:L:96:VAL:HG23	1.87	0.56
13:M:32:GLU:OE1	13:M:64:TRP:HZ2	1.89	0.56
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.71	0.56
1:A:1329:A:P	13:M:28:ALA:HB3	2.46	0.56
1:A:433:C:H2'	1:A:434:U:H3	1.71	0.56
1:A:539:A:H2'	1:A:540:G:H8	1.71	0.56
3:C:131:ARG:HG2	3:C:135:LYS:CE	2.34	0.56
3:C:64:VAL:CG2	3:C:99:VAL:HG11	2.32	0.56
9:I:127:LYS:HB2	13:M:126:LYS:HZ1	1.68	0.56
1:A:1250:A:C4'	9:I:68:GLY:H	2.14	0.56
11:K:67:ASP:OD1	11:K:71:LYS:HE3	2.06	0.56
13:M:73:GLU:O	13:M:76:ALA:HB3	2.05	0.56
1:A:1121:U:H2'	1:A:1122:U:H6	1.69	0.56
1:A:1288:A:H2'	1:A:1289:A:H8	1.71	0.56
2:B:25:ASN:ND2	2:B:27:LYS:H	2.03	0.56
3:C:155:GLY:O	3:C:156:ARG:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:ARG:HG2	8:H:85:ARG:N	2.20	0.56
9:I:79:LEU:HD22	9:I:83:ARG:HG3	1.88	0.56
13:M:49:THR:HG22	13:M:51:ALA:N	2.18	0.56
19:S:16:LEU:O	19:S:20:LEU:HG	2.05	0.56
1:A:1133:G:H2'	1:A:1134:G:C8	2.38	0.56
1:A:1228:C:H4'	13:M:116:THR:HA	1.87	0.56
1:A:1291:G:H4'	9:I:38:GLN:O	2.04	0.56
1:A:1497:G:O2'	1:A:1498:U:H5'	2.06	0.56
1:A:454:C:H2'	1:A:455:C:H5'	1.88	0.56
1:A:968:A:H4'	1:A:969:A:OP2	2.06	0.56
2:B:121:LEU:HB3	2:B:127:ILE:HG23	1.87	0.56
2:B:23:ARG:HH12	2:B:191:ASP:HA	1.69	0.56
3:C:190:ARG:HH11	3:C:190:ARG:CB	2.19	0.56
7:G:56:GLN:NE2	7:G:56:GLN:H	2.04	0.56
9:I:10:ARG:HD2	9:I:11:LYS:H	1.71	0.56
1:A:1250:A:H4'	9:I:68:GLY:CA	2.36	0.56
9:I:7:THR:HG22	9:I:8:GLY:N	2.20	0.56
10:J:94:VAL:CG1	10:J:95:GLU:N	2.69	0.56
15:O:4:THR:HB	15:O:6:GLU:OE2	2.05	0.56
1:A:1014:A:C2	1:A:1219:U:H1'	2.41	0.56
1:A:218:C:H2'	1:A:219:C:C6	2.40	0.56
1:A:475:G:H2'	1:A:476:G:C8	2.41	0.56
3:C:21:ARG:HH11	3:C:21:ARG:HG2	1.71	0.56
13:M:77:ASN:O	13:M:80:ARG:HB2	2.06	0.56
19:S:80:TYR:O	19:S:82:GLY:N	2.39	0.56
1:A:1316:G:N2	1:A:1318:A:H3'	2.21	0.55
1:A:420:U:H2'	1:A:422:C:C5	2.41	0.55
1:A:765:G:H1	1:A:812:C:H2'	1.70	0.55
3:C:123:GLN:O	3:C:128:PHE:HB2	2.07	0.55
5:E:80:ILE:HD11	5:E:91:LEU:HD12	1.88	0.55
7:G:138:LYS:C	7:G:138:LYS:HD3	2.27	0.55
10:J:49:VAL:O	10:J:60:ARG:O	2.24	0.55
16:P:81:ARG:HG3	16:P:83:GLU:HG2	1.88	0.55
1:A:353:A:H5'	1:A:353:A:C8	2.42	0.55
1:A:812:C:O2'	1:A:813:U:OP2	2.25	0.55
2:B:33:TYR:HB3	2:B:41:ILE:O	2.06	0.55
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.71	0.55
1:A:1007:C:O2'	1:A:1008:C:H5'	2.06	0.55
1:A:1126:U:H2'	1:A:1127:G:O4'	2.06	0.55
1:A:547:A:H4'	1:A:548:G:O5'	2.06	0.55
1:A:60:A:H4'	1:A:61:G:O5'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:ILE:CG2	3:C:168:ALA:HB3	2.37	0.55
6:F:33:TYR:CD1	6:F:75:LEU:HD23	2.41	0.55
8:H:119:LEU:HB3	8:H:123:GLU:HB2	1.89	0.55
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.07	0.55
12:L:38:THR:O	12:L:79:GLU:HG3	2.07	0.55
12:L:59:ARG:NE	12:L:65:GLU:HG3	2.22	0.55
13:M:78:ILE:O	13:M:81:LEU:HD23	2.06	0.55
17:Q:81:ARG:O	17:Q:81:ARG:HG3	2.07	0.55
1:A:1222:G:P	19:S:77:THR:HG21	2.46	0.55
1:A:624:C:H4'	16:P:11:SER:OG	2.06	0.55
5:E:41:VAL:HG13	5:E:113:ALA:HA	1.87	0.55
12:L:42:THR:HG21	12:L:52:LEU:HB3	1.87	0.55
1:A:1331:G:HO2'	1:A:1332:A:P	2.29	0.55
1:A:424:G:O2'	1:A:425:G:H5'	2.05	0.55
4:D:148:VAL:HG11	4:D:158:ILE:HD13	1.89	0.55
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.07	0.55
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.87	0.55
13:M:115:LYS:N	13:M:115:LYS:HD3	2.22	0.55
1:A:56:U:H2'	1:A:57:G:C8	2.42	0.55
1:A:746:A:O2'	1:A:747:C:H5'	2.07	0.55
4:D:162:LEU:HD13	4:D:181:MET:CG	2.37	0.55
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.42	0.55
12:L:17:LYS:HA	12:L:17:LYS:HE3	1.88	0.55
17:Q:93:GLN:O	17:Q:96:GLN:HB3	2.07	0.55
20:T:100:ILE:O	20:T:100:ILE:HG12	2.06	0.55
1:A:1347:G:O2'	1:A:1348:U:P	2.64	0.55
1:A:45:U:H2'	1:A:46:G:C8	2.42	0.55
1:A:80:G:C3'	1:A:81:U:H5"	2.37	0.55
5:E:80:ILE:H	5:E:80:ILE:HD12	1.72	0.55
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.41	0.55
9:I:40:LEU:O	9:I:42:ARG:N	2.40	0.55
11:K:79:SER:HB3	11:K:104:GLN:HB3	1.89	0.55
1:A:1048:G:H5"	14:N:3:ARG:HB3	1.89	0.55
20:T:36:LEU:HD12	20:T:62:LEU:HD12	1.88	0.55
1:A:357:G:O2'	1:A:358:U:H5'	2.06	0.55
1:A:984:C:H2'	1:A:985:C:H6	1.72	0.55
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.31	0.55
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.89	0.55
1:A:192:U:H4'	20:T:57:ARG:HD2	1.89	0.55
1:A:437:U:C2'	1:A:438:G:H5'	2.37	0.55
3:C:92:ALA:HA	3:C:95:THR:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:VAL:HG22	6:F:41:GLU:N	2.21	0.55
10:J:22:LYS:CE	10:J:90:LEU:HB2	2.36	0.55
10:J:42:THR:HG23	10:J:67:THR:C	2.28	0.55
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.41	0.55
19:S:51:VAL:O	19:S:58:VAL:HG22	2.07	0.55
1:A:191:G:C4	20:T:105:SER:HB3	2.42	0.55
1:A:444:C:H2'	1:A:491:G:N2	2.22	0.55
3:C:64:VAL:H	3:C:99:VAL:HB	1.71	0.55
5:E:152:ARG:C	8:H:64:LYS:HZ1	2.10	0.55
10:J:57:LYS:HE3	10:J:58:ASP:OD2	2.06	0.55
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.06	0.55
20:T:50:GLU:HG3	20:T:100:ILE:HB	1.89	0.55
20:T:70:SER:HA	20:T:73:HIS:CD2	2.42	0.55
1:A:1032:G:H2'	1:A:1033:G:H8	1.72	0.54
1:A:954:G:H2'	1:A:955:U:H6	1.72	0.54
2:B:15:VAL:CG2	2:B:209:ARG:HG3	2.37	0.54
3:C:35:GLU:HG3	3:C:95:THR:HG21	1.90	0.54
10:J:51:ARG:NE	10:J:61:GLU:HB2	2.23	0.54
14:N:26:ARG:CZ	14:N:47:LEU:HD21	2.36	0.54
18:R:36:ASN:HD21	18:R:38:GLU:HG2	1.70	0.54
1:A:370:C:O2'	1:A:371:G:H5'	2.06	0.54
1:A:818:G:C3'	1:A:819:A:C5'	2.85	0.54
2:B:15:VAL:O	2:B:16:HIS:O	2.26	0.54
3:C:64:VAL:HG12	3:C:66:VAL:HG23	1.88	0.54
13:M:125:ARG:HD2	13:M:126:LYS:N	2.22	0.54
20:T:96:GLY:O	20:T:97:ALA:HB3	2.06	0.54
1:A:1010:G:O2'	1:A:1011:G:H5'	2.07	0.54
1:A:1095:U:H2'	1:A:1096:C:C6	2.42	0.54
1:A:190(I):G:O2'	1:A:190(J):U:H5'	2.07	0.54
1:A:485:G:O2'	1:A:486:U:P	2.65	0.54
1:A:868:C:H2'	1:A:869:G:O4'	2.08	0.54
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.90	0.54
3:C:23:TYR:CG	3:C:24:ALA:N	2.75	0.54
8:H:82:HIS:O	8:H:83:ILE:HB	2.06	0.54
1:A:399:G:H2'	1:A:400:C:C6	2.42	0.54
1:A:948:C:P	13:M:106:ASN:O	2.66	0.54
6:F:19:LEU:HD23	6:F:19:LEU:C	2.26	0.54
7:G:12:LEU:H	7:G:12:LEU:HD12	1.72	0.54
12:L:110:VAL:O	12:L:122:THR:HG21	2.06	0.54
12:L:56:ALA:O	12:L:67:THR:HA	2.08	0.54
1:A:1021:G:H2'	1:A:1022:G:O4'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1370:G:O2'	1:A:1371:G:H5'	2.08	0.54
1:A:1347:G:H2'	1:A:1373:G:H1	1.71	0.54
1:A:17:U:H2'	1:A:18:C:C6	2.42	0.54
3:C:191:THR:HG23	3:C:192:THR:H	1.73	0.54
7:G:23:VAL:O	7:G:27:ILE:HG13	2.07	0.54
12:L:34:ARG:O	12:L:61:THR:HG23	2.07	0.54
17:Q:66:SER:OG	17:Q:69:LYS:HB3	2.08	0.54
1:A:1250:A:H2'	1:A:1251:A:C8	2.43	0.54
1:A:1483:A:H2'	1:A:1484:C:O4'	2.08	0.54
3:C:188:LEU:HD21	3:C:195:VAL:HG11	1.89	0.54
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.90	0.54
6:F:25:ILE:HD12	6:F:82:ARG:HH11	1.73	0.54
9:I:82:ALA:O	9:I:86:VAL:HG23	2.08	0.54
12:L:54:LYS:N	12:L:54:LYS:HD2	2.22	0.54
1:A:1165:C:O2'	1:A:1166:G:H5'	2.07	0.54
1:A:190:C:H2'	1:A:190(A):C:H6	1.73	0.54
3:C:26:LYS:H	3:C:26:LYS:CE	2.13	0.54
3:C:51:GLY:O	3:C:53:ALA:N	2.41	0.54
4:D:3:ARG:NH2	4:D:71:SER:HB3	2.22	0.54
10:J:48:THR:HG1	10:J:62:HIS:CD2	2.25	0.54
10:J:5:ARG:HA	10:J:73:ASP:OD1	2.07	0.54
12:L:83:VAL:CG1	12:L:100:ILE:HG23	2.37	0.54
1:A:1286:A:H4'	21:U:25:LYS:HE2	1.89	0.54
1:A:1002:G:H2'	1:A:1003:G:C8	2.42	0.54
2:B:55:PHE:CD2	2:B:58:ILE:HD12	2.41	0.54
2:B:73:THR:HG23	2:B:96:ARG:NH2	2.21	0.54
3:C:91:LEU:HD11	3:C:99:VAL:CG2	2.37	0.54
8:H:4:ASP:OD2	8:H:7:ALA:HB2	2.08	0.54
9:I:95:LYS:O	9:I:99:LEU:HD23	2.08	0.54
17:Q:17:LYS:HA	17:Q:46:ASP:O	2.08	0.54
1:A:1312:G:O2'	1:A:1313:U:H5'	2.08	0.54
1:A:477:G:N3	1:A:477:G:H2'	2.22	0.54
1:A:939:G:H5"	7:G:102:ARG:HH22	1.71	0.54
2:B:12:GLU:CD	2:B:213:LEU:HD11	2.28	0.54
2:B:91:PRO:HG3	2:B:154:LEU:CB	2.35	0.54
3:C:204:LEU:O	3:C:204:LEU:HD12	2.07	0.54
3:C:77:ILE:HG22	3:C:81:GLY:HA2	1.89	0.54
1:A:737:A:H1'	6:F:73:ASN:OD1	2.07	0.54
8:H:110:ALA:HB3	8:H:121:ASP:HB3	1.89	0.54
9:I:26:VAL:HA	9:I:61:ALA:O	2.07	0.54
11:K:16:SER:HA	11:K:79:SER:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:11:VAL:HG22	17:Q:29:HIS:CD2	2.43	0.54
13:M:107:ALA:HB3	13:M:111:LYS:HD2	1.90	0.54
19:S:45:VAL:HA	19:S:62:ILE:HG13	1.89	0.54
1:A:1160:G:O2'	1:A:1161:C:H5'	2.08	0.54
3:C:34:LEU:HD23	3:C:34:LEU:O	2.08	0.54
10:J:12:ASP:O	10:J:15:THR:HG22	2.07	0.54
11:K:76:GLY:O	11:K:78:GLN:HG3	2.08	0.54
12:L:27:LEU:HG	12:L:28:LYS:N	2.22	0.54
13:M:11:ARG:CG	13:M:12:ASN:N	2.71	0.54
15:O:9:GLN:O	15:O:13:GLN:NE2	2.41	0.54
1:A:107:G:C2'	1:A:108:G:H5'	2.39	0.53
1:A:701:C:H5"	1:A:702:A:H3'	1.89	0.53
8:H:91:ARG:HG3	12:L:7:ILE:HG13	1.90	0.53
12:L:89:ARG:NH2	12:L:97:ARG:HE	2.06	0.53
12:L:89:ARG:HH22	12:L:97:ARG:HH21	1.56	0.53
13:M:40:ASN:HD22	13:M:41:PRO:N	2.05	0.53
15:O:30:ALA:HA	15:O:85:LEU:HD11	1.91	0.53
16:P:26:ARG:HD3	16:P:31:LYS:H	1.72	0.53
20:T:56:MET:HG2	20:T:84:LEU:HD13	1.89	0.53
1:A:1151:A:O2'	1:A:1152:A:H8	1.91	0.53
1:A:1182:G:H4'	1:A:1183:A:C5'	2.37	0.53
1:A:1368:G:O2'	1:A:1369:C:H5'	2.08	0.53
2:B:114:ARG:HH12	2:B:118:LEU:HD21	1.70	0.53
2:B:77:ALA:HB2	2:B:211:ILE:HD12	1.90	0.53
3:C:52:LEU:HD23	3:C:52:LEU:N	2.23	0.53
6:F:28:ARG:HA	6:F:31:GLU:OE1	2.08	0.53
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.72	0.53
9:I:4:TYR:CZ	9:I:88:TYR:HD1	2.27	0.53
13:M:22:ILE:HD12	13:M:25:ILE:HD12	1.89	0.53
13:M:3:ARG:HH21	13:M:7:VAL:HG12	1.73	0.53
1:A:1023:G:N3	1:A:1023:G:H2'	2.22	0.53
1:A:994:A:N3	1:A:994:A:H2'	2.22	0.53
3:C:91:LEU:CD1	3:C:99:VAL:HG22	2.38	0.53
9:I:8:GLY:HA2	9:I:79:LEU:CD1	2.37	0.53
1:A:666:G:H5'	1:A:726:C:H1'	1.91	0.53
2:B:230:VAL:HG12	2:B:231:GLU:N	2.23	0.53
4:D:122:ARG:HA	4:D:122:ARG:HE	1.73	0.53
10:J:10:GLY:N	10:J:16:LEU:HD11	2.19	0.53
20:T:39:LYS:HD3	20:T:55:ILE:HD13	1.90	0.53
21:U:24:ARG:HH11	21:U:24:ARG:CB	2.17	0.53
1:A:1271:G:H2'	1:A:1272:G:H8	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:LYS:O	2:B:9:GLU:HB3	2.08	0.53
3:C:52:LEU:CD2	3:C:118:GLN:HE22	2.17	0.53
5:E:7:GLU:O	5:E:34:VAL:HA	2.08	0.53
5:E:43:LEU:HB2	5:E:136:MET:HE2	1.90	0.53
1:A:938:A:H5'	7:G:76:ARG:HH21	1.73	0.53
10:J:22:LYS:HZ3	10:J:91:PRO:HD3	1.73	0.53
11:K:79:SER:CB	11:K:104:GLN:HB3	2.38	0.53
1:A:1003(A):G:C5	1:A:1004:A:H1'	2.44	0.53
1:A:475:G:H2'	1:A:476:G:H8	1.74	0.53
1:A:594:G:C2'	1:A:595:G:H5'	2.38	0.53
5:E:122:GLU:O	5:E:123:LEU:HD23	2.08	0.53
5:E:9:LYS:HG3	5:E:112:LEU:HD11	1.90	0.53
6:F:48:LEU:HD13	6:F:52:ILE:HG13	1.90	0.53
14:N:41:ARG:HG3	14:N:42:ILE:N	2.24	0.53
17:Q:59:ILE:CG2	17:Q:71:PHE:HB3	2.39	0.53
1:A:416:G:C6	1:A:417:C:H5	2.27	0.53
1:A:409:G:H22	1:A:434:U:H6	1.56	0.53
1:A:485:G:C2'	1:A:486:U:OP2	2.57	0.53
1:A:81:U:H6	1:A:81:U:H5'	1.73	0.53
2:B:25:ASN:HD22	2:B:27:LYS:H	1.57	0.53
3:C:79:ARG:HE	3:C:82:GLU:HG2	1.73	0.53
6:F:21:LEU:O	6:F:24:GLU:HB3	2.09	0.53
9:I:36:TYR:HD2	9:I:37:PHE:CE2	2.27	0.53
9:I:97:LYS:HG2	9:I:102:LEU:CD1	2.39	0.53
1:A:1124:G:C5'	10:J:35:SER:O	2.54	0.53
11:K:115:PRO:C	11:K:117:ASN:H	2.11	0.53
14:N:14:PRO:O	14:N:15:LYS:CB	2.55	0.53
16:P:28:ARG:HG3	16:P:29:ASP:OD2	2.08	0.53
21:U:24:ARG:CD	21:U:24:ARG:H	2.20	0.53
1:A:335:C:H2'	1:A:336:C:H6	1.74	0.53
3:C:190:ARG:HB3	3:C:190:ARG:NH1	2.22	0.53
7:G:18:TYR:HD1	7:G:18:TYR:H	1.57	0.53
8:H:10:LEU:HD12	8:H:85:ARG:HG2	1.90	0.53
14:N:9:LYS:O	14:N:11:LYS:N	2.42	0.53
15:O:88:ARG:HB2	15:O:88:ARG:CZ	2.38	0.53
1:A:954:G:H21	1:A:1227:A:H62	1.56	0.53
1:A:1407:C:O2'	1:A:1408:A:H5'	2.09	0.53
1:A:1487:G:O2'	1:A:1488:G:H5'	2.08	0.53
1:A:412:A:C4	1:A:413:G:C2'	2.85	0.53
1:A:791:G:H2'	1:A:792:A:H5"	1.91	0.53
1:A:911:U:H2'	1:A:912:C:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:LYS:O	2:B:137:ARG:HG3	2.09	0.53
2:B:185:ILE:HD12	2:B:185:ILE:H	1.74	0.53
2:B:88:ALA:C	2:B:90:MET:H	2.11	0.53
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.39	0.53
13:M:40:ASN:ND2	13:M:42:ALA:H	2.07	0.53
15:O:3:ILE:HD11	15:O:38:ARG:HG3	1.91	0.53
17:Q:68:ARG:HH11	17:Q:68:ARG:CG	2.19	0.53
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.08	0.53
3:C:40:ARG:O	3:C:44:GLU:HG3	2.09	0.53
4:D:170:VAL:HG21	4:D:176:LEU:HD22	1.91	0.53
1:A:1346:A:C4	7:G:10:ARG:NH2	2.77	0.53
9:I:47:LEU:C	9:I:49:PRO:HD2	2.29	0.53
9:I:48:GLU:N	9:I:49:PRO:CD	2.72	0.53
16:P:67:THR:HG22	16:P:68:ASP:N	2.24	0.53
22:X:39:A:C2'	22:X:40:U:H5'	2.38	0.53
1:A:1064:G:H4'	1:A:1065:U:H5"	1.90	0.52
1:A:404:U:H2'	1:A:405:U:C6	2.45	0.52
1:A:455:C:O2'	1:A:456:C:H5'	2.08	0.52
2:B:7:VAL:HG11	2:B:221:LEU:CD2	2.30	0.52
3:C:35:GLU:CD	3:C:95:THR:HG21	2.28	0.52
4:D:127:THR:HG23	4:D:147:ALA:HB3	1.91	0.52
11:K:12:ARG:H	11:K:13:GLN:HE21	1.55	0.52
13:M:78:ILE:HA	13:M:81:LEU:CD2	2.39	0.52
17:Q:60:ILE:HD13	17:Q:61:GLU:N	2.23	0.52
18:R:47:THR:HA	18:R:83:GLU:HB2	1.90	0.52
18:R:86:VAL:O	18:R:87:ARG:CB	2.51	0.52
1:A:1065:U:H4'	1:A:1066:C:O5'	2.09	0.52
1:A:1527:C:O2'	1:A:1528:U:H5'	2.09	0.52
1:A:266:G:H5"	1:A:268:C:N4	2.13	0.52
1:A:838:G:H2'	1:A:839:U:C5'	2.34	0.52
3:C:39:ILE:CD1	3:C:57:ILE:HD13	2.38	0.52
4:D:156:GLU:HG2	4:D:160:GLN:NE2	2.24	0.52
4:D:36:ARG:N	4:D:37:PRO:HD3	2.21	0.52
9:I:11:LYS:HG2	9:I:11:LYS:O	2.09	0.52
9:I:92:TYR:O	9:I:96:LEU:HD13	2.09	0.52
10:J:39:PRO:O	10:J:69:ASN:O	2.27	0.52
10:J:80:LYS:HA	10:J:83:GLU:OE2	2.10	0.52
12:L:93:LEU:O	12:L:96:VAL:HG23	2.09	0.52
13:M:13:LYS:O	13:M:45:VAL:HG23	2.09	0.52
13:M:81:LEU:H	13:M:81:LEU:CD2	2.21	0.52
14:N:45:ARG:HG3	14:N:45:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:104:LYS:HD3	17:Q:104:LYS:O	2.10	0.52
1:A:1454:G:O2'	1:A:1455:G:H5'	2.09	0.52
1:A:411:A:O4'	1:A:429:U:H5	1.92	0.52
1:A:724:G:O2'	1:A:725:G:H5'	2.10	0.52
1:A:860:A:H2'	1:A:861:G:O4'	2.09	0.52
7:G:32:ARG:O	7:G:33:ASP:HB2	2.09	0.52
10:J:86:MET:HA	10:J:86:MET:CE	2.39	0.52
12:L:40:VAL:HG21	12:L:78:GLN:O	2.10	0.52
15:O:70:LEU:HD11	15:O:77:ARG:HB2	1.91	0.52
15:O:25:THR:HG21	15:O:70:LEU:HD23	1.92	0.52
1:A:1004:A:H5"	1:A:1025:U:O4	2.09	0.52
1:A:1152:A:H2'	1:A:1153:C:C6	2.45	0.52
1:A:332:G:O2'	1:A:333:G:H5'	2.09	0.52
1:A:538:G:H2'	1:A:539:A:C8	2.44	0.52
3:C:136:GLN:O	3:C:139:GLN:HB2	2.08	0.52
3:C:172:ARG:HB3	3:C:172:ARG:HH11	1.74	0.52
3:C:207:VAL:HG12	3:C:208:ILE:N	2.24	0.52
6:F:46:ARG:HE	6:F:47:ARG:HH21	1.58	0.52
7:G:50:ILE:O	7:G:54:THR:HB	2.09	0.52
10:J:8:LEU:HB2	10:J:70:ARG:CB	2.33	0.52
15:O:14:GLU:HG3	15:O:15:PHE:CD1	2.44	0.52
15:O:82:ILE:HD13	15:O:88:ARG:NH2	2.24	0.52
1:A:377:G:OP1	16:P:3:LYS:HD3	2.10	0.52
18:R:37:VAL:HG12	18:R:41:LYS:HD3	1.91	0.52
18:R:53:ARG:HG2	18:R:63:GLN:OE1	2.09	0.52
1:A:1405:G:O2'	1:A:1406:U:H5'	2.09	0.52
1:A:1441:G:H4'	1:A:1442:G:C5	2.44	0.52
1:A:1454:G:H2'	1:A:1455:G:H8	1.75	0.52
2:B:185:ILE:HD12	2:B:185:ILE:N	2.24	0.52
3:C:174:PRO:HB2	3:C:177:THR:HG21	1.90	0.52
6:F:33:TYR:CG	6:F:75:LEU:HD23	2.44	0.52
7:G:136:LYS:NZ	7:G:136:LYS:HB3	2.24	0.52
1:A:740:U:O2'	1:A:741:G:H5'	2.09	0.52
1:A:975:A:O5'	1:A:976:G:H5'	2.09	0.52
1:A:992:U:O2'	1:A:993:G:OP2	2.26	0.52
4:D:3:ARG:HH21	4:D:71:SER:HB3	1.74	0.52
1:A:921:U:O2'	5:E:19:MET:O	2.21	0.52
7:G:51:GLN:OE1	7:G:51:GLN:HA	2.09	0.52
9:I:27:THR:OG1	9:I:62:TYR:HD1	1.92	0.52
13:M:40:ASN:HD22	13:M:41:PRO:CD	2.23	0.52
20:T:45:GLN:C	20:T:47:GLY:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1317:C:OP1	14:N:17:LYS:HG2	2.09	0.52
1:A:603:U:H2'	1:A:604:G:H8	1.75	0.52
1:A:789:U:H2'	1:A:791:G:OP2	2.10	0.52
2:B:23:ARG:HH11	2:B:24:TRP:HA	1.75	0.52
1:A:738:C:P	6:F:92:LYS:HE3	2.50	0.52
7:G:125:MET:O	7:G:129:GLU:HG2	2.10	0.52
10:J:32:ALA:CB	10:J:76:ASN:HD22	2.22	0.52
1:A:521:G:OP1	12:L:73:GLU:O	2.28	0.52
18:R:26:LEU:HD21	18:R:39:VAL:HG22	1.91	0.52
1:A:1090:U:H2'	1:A:1091:U:H6	1.74	0.52
1:A:1144:G:H21	1:A:1146:A:H62	1.57	0.52
1:A:1225:A:H5'	1:A:1226:C:OP2	2.10	0.52
1:A:184:G:H2'	1:A:185:A:H8	1.75	0.52
1:A:665:A:C1'	1:A:733:A:H1'	2.40	0.52
1:A:956:U:O2'	1:A:957:U:H5'	2.10	0.52
1:A:983:A:H2	1:A:984:C:C6	2.28	0.52
2:B:168:THR:OG1	2:B:192:SER:HB3	2.10	0.52
2:B:28:PHE:CD2	2:B:190:THR:HA	2.45	0.52
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.75	0.52
3:C:47:LEU:N	3:C:47:LEU:HD12	2.25	0.52
3:C:61:ALA:O	3:C:62:ASP:HB2	2.10	0.52
12:L:56:ALA:HB2	12:L:70:ILE:HD11	1.92	0.52
17:Q:63:ARG:O	17:Q:65:ILE:HD12	2.10	0.52
1:A:1244:C:O2'	1:A:1245:A:H5'	2.10	0.52
1:A:222:U:H2'	1:A:223:U:C6	2.45	0.52
1:A:382:A:H2'	1:A:383:A:C8	2.45	0.52
1:A:976:G:C8	1:A:1358:U:C2	2.97	0.52
2:B:144:ARG:O	2:B:147:LYS:N	2.41	0.52
2:B:116:GLU:HG2	2:B:153:ARG:HH12	1.75	0.52
3:C:157:ILE:CD1	3:C:166:GLU:HB2	2.40	0.52
3:C:60:ALA:O	3:C:61:ALA:HB2	2.10	0.52
4:D:57:ARG:NH1	4:D:57:ARG:HG3	2.25	0.52
8:H:80:ILE:HG22	8:H:80:ILE:O	2.08	0.52
20:T:56:MET:HE1	20:T:104:LEU:HG	1.92	0.52
1:A:1005:A:H2'	1:A:1006:C:H5'	1.92	0.52
1:A:1015:A:H2'	1:A:1016:A:C8	2.45	0.52
7:G:49:ILE:HG22	7:G:49:ILE:O	2.10	0.52
9:I:57:GLY:O	9:I:58:ARG:HG2	2.10	0.52
1:A:1064:G:C4'	1:A:1065:U:H5'	2.40	0.51
1:A:554:C:H2'	1:A:555:C:H6	1.75	0.51
3:C:58:GLU:OE2	10:J:92:THR:HG21	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:G:O2'	4:D:116:GLN:HG3	2.09	0.51
4:D:17:VAL:HG12	4:D:18:LYS:N	2.25	0.51
16:P:57:ARG:NH1	16:P:79:VAL:O	2.43	0.51
18:R:19:LYS:NZ	18:R:55:ARG:HD2	2.25	0.51
18:R:36:ASN:HD22	18:R:36:ASN:C	2.13	0.51
1:A:1422:G:O2'	1:A:1423:G:H5'	2.11	0.51
1:A:1438:G:H2'	1:A:1439:C:C6	2.45	0.51
1:A:1510:U:H2'	1:A:1511:G:C8	2.45	0.51
1:A:113:G:H1'	1:A:354:G:C5'	2.40	0.51
1:A:418:C:O5'	1:A:418:C:H6	1.92	0.51
1:A:594:G:H2'	1:A:595:G:H5'	1.91	0.51
1:A:848:C:H2'	1:A:849:C:C6	2.45	0.51
1:A:953:G:H1'	13:M:125:ARG:CA	2.41	0.51
2:B:80:ILE:CD1	2:B:80:ILE:H	2.20	0.51
4:D:3:ARG:HG3	4:D:118:ARG:NH1	2.25	0.51
1:A:1004:A:N7	1:A:1037:C:N3	2.59	0.51
1:A:1231:G:O3'	9:I:126:SER:HB2	2.11	0.51
1:A:1286:A:C8	1:A:1287:A:H4'	2.45	0.51
1:A:1331:G:O2'	1:A:1332:A:P	2.67	0.51
1:A:603:U:H2'	1:A:604:G:C8	2.46	0.51
1:A:722:A:N3	1:A:722:A:H3'	2.26	0.51
2:B:91:PRO:HG2	2:B:155:LEU:CD2	2.40	0.51
4:D:100:ARG:HH12	4:D:137:SER:HB3	1.75	0.51
8:H:39:LEU:HD12	8:H:44:PHE:HB2	1.92	0.51
9:I:31:GLN:HB3	9:I:35:GLU:CG	2.41	0.51
11:K:48:ILE:HD11	11:K:67:ASP:HB2	1.91	0.51
13:M:14:ARG:NH1	13:M:16:ASP:OD2	2.43	0.51
1:A:1320:C:OP1	19:S:70:LYS:HE3	2.11	0.51
1:A:1007:C:N4	1:A:1022:G:H22	2.09	0.51
1:A:1131:G:H2'	1:A:1132:C:C6	2.45	0.51
1:A:1137:C:H4'	1:A:1138:G:N1	2.25	0.51
1:A:142:G:N3	1:A:196:A:H2	2.08	0.51
1:A:640:A:O2'	1:A:641:U:H5'	2.11	0.51
1:A:839:U:C2'	1:A:839:U:O2	2.58	0.51
6:F:43:LEU:N	6:F:43:LEU:HD22	2.26	0.51
1:A:267:C:OP2	17:Q:67:LYS:HD2	2.10	0.51
17:Q:79:SER:O	17:Q:80:GLY:O	2.29	0.51
1:A:945:G:H2'	1:A:945:G:N3	2.25	0.51
3:C:127:ARG:HG3	3:C:127:ARG:NH1	2.24	0.51
3:C:178:LEU:O	3:C:179:ARG:CB	2.58	0.51
6:F:78:GLU:O	6:F:81:ILE:HG13	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:25:GLU:C	10:J:27:ALA:H	2.13	0.51
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.25	0.51
16:P:20:VAL:CG1	16:P:32:TYR:CB	2.89	0.51
18:R:26:LEU:HD11	18:R:39:VAL:HG23	1.92	0.51
19:S:36:ARG:NH2	19:S:75:ALA:O	2.43	0.51
20:T:10:LEU:HD12	20:T:12:ALA:HB3	1.92	0.51
1:A:841:U:H3'	1:A:848:C:H5'	1.92	0.51
2:B:102:LEU:HD12	2:B:102:LEU:N	2.25	0.51
1:A:559:A:OP2	5:E:126:ARG:NH2	2.43	0.51
8:H:112:LEU:CD2	8:H:112:LEU:N	2.73	0.51
9:I:111:ARG:HD3	9:I:112:LYS:C	2.30	0.51
10:J:34:VAL:HG12	10:J:35:SER:N	2.25	0.51
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.76	0.51
10:J:76:ASN:O	10:J:78:ASN:N	2.43	0.51
11:K:58:PRO:HB2	11:K:93:GLN:HG3	1.93	0.51
23:Y:3:G:H2'	23:Y:4:U:C5'	2.26	0.51
1:A:1142:G:H2'	1:A:1143:G:O4'	2.10	0.51
1:A:1494:G:O2'	1:A:1495:U:H5'	2.10	0.51
1:A:285:G:O2'	1:A:286:G:H5'	2.10	0.51
1:A:556:C:OP2	12:L:20:LYS:HE3	2.10	0.51
4:D:119:GLN:HG2	4:D:123:HIS:NE2	2.26	0.51
4:D:17:VAL:HG11	4:D:197:PRO:CB	2.40	0.51
4:D:8:VAL:HG11	4:D:21:LEU:HB2	1.92	0.51
1:A:711:G:P	6:F:54:LYS:NZ	2.84	0.51
9:I:51:ARG:CG	9:I:56:LEU:HD12	2.39	0.51
19:S:63:THR:HG22	19:S:64:GLU:H	1.75	0.51
1:A:1272:G:O2'	1:A:1273:G:H5'	2.11	0.51
2:B:221:LEU:O	2:B:221:LEU:HD13	2.10	0.51
6:F:4:TYR:HD1	6:F:92:LYS:HA	1.76	0.51
7:G:80:VAL:O	7:G:81:GLY:C	2.50	0.51
18:R:16:PRO:O	18:R:17:SER:HB3	2.11	0.51
1:A:1216:G:O2'	1:A:1217:C:H5'	2.10	0.51
1:A:1346:A:O4'	1:A:1348:U:C6	2.64	0.51
1:A:839:U:C5'	1:A:840:C:H5	2.21	0.51
2:B:45:GLN:O	2:B:48:MET:HB2	2.11	0.51
3:C:138:VAL:HG22	3:C:151:VAL:HG23	1.93	0.51
3:C:14:ILE:HG22	3:C:15:THR:N	2.19	0.51
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.93	0.51
6:F:30:LEU:HB3	6:F:35:ALA:CB	2.41	0.51
1:A:1195:C:H3'	1:A:1196:U:C5'	2.41	0.51
1:A:1323:G:H2'	1:A:1324:A:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:G:O2'	1:A:227:G:H5'	2.11	0.51
1:A:551:U:H2'	1:A:552:U:C6	2.46	0.51
4:D:70:ILE:HG22	4:D:71:SER:N	2.26	0.51
9:I:108:VAL:CG1	9:I:109:VAL:H	2.08	0.51
10:J:18:ALA:O	10:J:22:LYS:HG3	2.11	0.51
10:J:9:ARG:HB3	10:J:9:ARG:CZ	2.41	0.51
12:L:41:ARG:CG	12:L:42:THR:H	1.98	0.51
12:L:89:ARG:HA	12:L:97:ARG:HA	1.92	0.51
18:R:46:GLU:CD	18:R:46:GLU:H	2.14	0.51
1:A:1326:C:H5"	21:U:12:LYS:NZ	2.25	0.51
23:Y:2:C:H2'	23:Y:3:G:C8	2.47	0.51
1:A:335:C:O2'	1:A:336:C:H5'	2.11	0.50
1:A:501:C:H2'	1:A:502:G:H8	1.76	0.50
1:A:813:U:OP1	1:A:904:C:H5'	2.10	0.50
1:A:961:U:O2'	1:A:962:C:H5'	2.12	0.50
3:C:112:SER:HB2	3:C:115:LEU:HD12	1.92	0.50
3:C:90:GLU:HA	3:C:93:LYS:CG	2.41	0.50
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.93	0.50
6:F:19:LEU:HD21	6:F:23:LYS:HD2	1.93	0.50
1:A:1333:A:H2'	1:A:1334:G:O4'	2.11	0.50
2:B:22:LYS:HD2	2:B:35:GLU:OE2	2.11	0.50
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.74	0.50
2:B:178:ARG:O	8:H:71:GLY:HA2	2.11	0.50
1:A:1128:C:C5'	9:I:16:ARG:HH12	2.24	0.50
13:M:40:ASN:C	13:M:40:ASN:HD22	2.15	0.50
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.93	0.50
1:A:974:A:OP2	14:N:41:ARG:NH1	2.44	0.50
16:P:10:GLY:HA3	16:P:14:ASN:O	2.11	0.50
16:P:20:VAL:CG1	16:P:21:VAL:N	2.73	0.50
17:Q:80:GLY:O	17:Q:81:ARG:HB3	2.11	0.50
19:S:35:SER:O	19:S:71:LEU:HD12	2.12	0.50
1:A:1145:C:O2'	1:A:1146:A:C8	2.62	0.50
1:A:457:C:H2'	1:A:458:C:H6	1.76	0.50
1:A:58:C:O2'	1:A:59:A:H5'	2.12	0.50
2:B:124:SER:OG	2:B:125:PRO:HD2	2.12	0.50
2:B:36:ARG:HD2	2:B:41:ILE:HD12	1.92	0.50
2:B:77:ALA:HB3	2:B:211:ILE:HD13	1.93	0.50
3:C:179:ARG:O	3:C:179:ARG:CG	2.60	0.50
3:C:79:ARG:HE	3:C:82:GLU:CB	2.23	0.50
5:E:151:LEU:HD23	8:H:79:VAL:HG22	1.93	0.50
6:F:1:MET:H3	6:F:1:MET:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:59:LEU:O	7:G:63:LYS:HG2	2.12	0.50
9:I:127:LYS:HB2	13:M:126:LYS:CE	2.41	0.50
17:Q:40:LYS:HD2	17:Q:42:TYR:CE1	2.46	0.50
19:S:30:LEU:O	19:S:31:ILE:HD13	2.11	0.50
21:U:17:THR:O	21:U:22:ARG:HD3	2.10	0.50
1:A:900:A:H2'	1:A:901:A:C8	2.46	0.50
3:C:147:LYS:HE2	3:C:205:GLY:N	2.26	0.50
7:G:20:ASP:OD2	7:G:63:LYS:NZ	2.43	0.50
7:G:92:SER:O	7:G:96:GLN:HB2	2.10	0.50
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.45	0.50
10:J:39:PRO:O	10:J:40:LEU:CB	2.55	0.50
10:J:32:ALA:HB2	10:J:76:ASN:ND2	2.26	0.50
12:L:28:LYS:O	12:L:29:GLY:C	2.49	0.50
16:P:39:TYR:CZ	16:P:41:PRO:HA	2.46	0.50
16:P:67:THR:CG2	16:P:68:ASP:N	2.74	0.50
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.11	0.50
1:A:1157:A:H4'	1:A:1158:C:O5'	2.11	0.50
1:A:1176:A:H2'	1:A:1177:G:H8	1.76	0.50
1:A:131:C:H2'	1:A:132:C:C6	2.45	0.50
1:A:242:C:C2'	1:A:243:A:H5'	2.41	0.50
3:C:132:ARG:HB3	3:C:132:ARG:NH1	2.26	0.50
3:C:147:LYS:HE2	3:C:205:GLY:H	1.77	0.50
3:C:91:LEU:HD11	3:C:99:VAL:N	2.23	0.50
6:F:48:LEU:HD13	6:F:52:ILE:CG1	2.42	0.50
9:I:85:LEU:HG	9:I:92:TYR:HD1	1.75	0.50
16:P:20:VAL:CG1	16:P:32:TYR:HB3	2.41	0.50
1:A:1310:G:N7	19:S:2:PRO:HD3	2.27	0.50
1:A:1062:U:H2'	1:A:1063:C:C6	2.47	0.50
1:A:1196:U:H5"	1:A:1197:G:H5'	1.93	0.50
1:A:57:G:H2'	1:A:58:C:C6	2.46	0.50
1:A:401:C:H1'	1:A:622:A:H1'	1.93	0.50
3:C:110:ASN:C	3:C:111:LEU:HD23	2.32	0.50
4:D:35:ARG:O	4:D:36:ARG:CB	2.60	0.50
5:E:144:THR:H	5:E:147:ASP:HB2	1.77	0.50
8:H:104:ARG:NH2	8:H:138:TRP:CZ3	2.79	0.50
1:A:1250:A:H5"	9:I:68:GLY:N	2.26	0.50
10:J:8:LEU:HD13	10:J:20:ALA:HB2	1.92	0.50
15:O:36:ILE:HA	15:O:59:MET:HE3	1.93	0.50
1:A:1283:G:O2'	1:A:1284:C:H5'	2.12	0.50
1:A:179:A:H2'	1:A:180:U:C6	2.47	0.50
1:A:868:C:O2'	1:A:869:G:H5'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:PHE:HD1	2:B:18:GLY:N	2.09	0.50
2:B:73:THR:CG2	2:B:96:ARG:HH21	2.20	0.50
3:C:191:THR:HG23	3:C:192:THR:N	2.27	0.50
5:E:15:ARG:HD2	5:E:15:ARG:O	2.11	0.50
7:G:69:VAL:O	7:G:69:VAL:HG12	2.12	0.50
10:J:8:LEU:CD2	10:J:96:ILE:HG12	2.42	0.50
16:P:22:THR:HA	16:P:33:ILE:HG13	1.94	0.50
17:Q:104:LYS:C	17:Q:104:LYS:HD3	2.32	0.50
1:A:1022:G:H2'	1:A:1023:G:H8	1.77	0.50
1:A:1406:U:O2'	1:A:1407:C:H5'	2.12	0.50
1:A:175:C:H2'	1:A:176:C:C6	2.39	0.50
1:A:218:C:H2'	1:A:219:C:H6	1.77	0.50
2:B:51:LEU:HD22	2:B:55:PHE:CE1	2.46	0.50
5:E:40:ARG:HH11	5:E:40:ARG:HG2	1.76	0.50
1:A:967:C:C4'	9:I:128:ARG:HG3	2.40	0.50
10:J:87:THR:O	10:J:87:THR:HG22	2.11	0.50
11:K:126:ARG:O	11:K:127:LYS:CB	2.59	0.50
12:L:117:ARG:O	12:L:119:LYS:O	2.30	0.50
12:L:92:ASP:C	12:L:93:LEU:HD23	2.32	0.50
13:M:59:TYR:O	13:M:63:THR:HB	2.11	0.50
14:N:6:LEU:C	14:N:8:GLU:H	2.14	0.50
19:S:36:ARG:HA	19:S:71:LEU:HB2	1.93	0.50
1:A:456:C:H2'	1:A:457:C:C6	2.47	0.50
1:A:477:G:C3'	1:A:478:A:H5"	2.41	0.50
1:A:51:A:H4'	1:A:52:G:C5'	2.42	0.50
1:A:662:G:O2'	1:A:836:G:H5'	2.12	0.50
3:C:179:ARG:CD	3:C:206:GLU:HG2	2.42	0.50
1:A:427:U:OP1	4:D:13:ARG:NH2	2.45	0.50
4:D:98:GLU:CG	4:D:189:PRO:HG3	2.37	0.50
7:G:72:ARG:HG2	7:G:142:GLU:OE1	2.12	0.50
18:R:47:THR:HG23	18:R:83:GLU:O	2.12	0.50
1:A:107:G:H2'	1:A:108:G:H5'	1.94	0.49
1:A:1120:G:H2'	1:A:1121:U:C6	2.47	0.49
1:A:1320:C:H41	19:S:37:ARG:HH11	1.58	0.49
1:A:404:U:H2'	1:A:405:U:H6	1.77	0.49
3:C:195:VAL:C	3:C:196:LEU:HD22	2.33	0.49
8:H:36:LEU:CD1	8:H:59:LEU:HD13	2.41	0.49
16:P:11:SER:HB2	16:P:14:ASN:HB3	1.93	0.49
19:S:40:ILE:HB	19:S:67:VAL:O	2.12	0.49
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.94	0.49
1:A:1116:C:O2'	1:A:1117:G:H5"	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:A:N3	1:A:1225:A:H2'	2.27	0.49
1:A:743:U:H2'	1:A:744:C:C6	2.47	0.49
2:B:52:GLU:CG	2:B:56:ARG:HH21	2.24	0.49
3:C:23:TYR:CD2	3:C:24:ALA:N	2.80	0.49
5:E:51:VAL:O	5:E:55:VAL:HG23	2.12	0.49
13:M:81:LEU:HA	13:M:84:ILE:HG12	1.94	0.49
16:P:26:ARG:HG2	16:P:27:LYS:N	2.27	0.49
16:P:43:LYS:HA	16:P:48:TRP:CB	2.42	0.49
1:A:1171:G:H2'	1:A:1172:C:C6	2.48	0.49
1:A:1512:U:O2'	1:A:1513:A:H5'	2.13	0.49
1:A:390:C:H2'	1:A:391:G:H8	1.75	0.49
3:C:139:GLN:O	3:C:143:GLU:N	2.42	0.49
7:G:20:ASP:OD1	7:G:22:LEU:HB3	2.12	0.49
9:I:10:ARG:HD2	9:I:11:LYS:N	2.27	0.49
9:I:65:VAL:HG21	9:I:73:GLN:HB3	1.92	0.49
10:J:22:LYS:CE	10:J:91:PRO:HD3	2.41	0.49
12:L:83:VAL:CG1	12:L:84:LEU:N	2.76	0.49
16:P:51:VAL:O	16:P:53:VAL:N	2.46	0.49
1:A:1047:G:O2'	1:A:1048:G:H5'	2.12	0.49
1:A:780:A:O2'	1:A:781:A:H5"	2.12	0.49
2:B:137:ARG:HB3	2:B:137:ARG:NH1	2.28	0.49
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.94	0.49
10:J:51:ARG:CZ	10:J:61:GLU:HB2	2.42	0.49
13:M:20:THR:C	13:M:22:ILE:H	2.15	0.49
20:T:49:ALA:HB3	20:T:99:LEU:HG	1.95	0.49
1:A:1417:G:H2'	1:A:1482:G:H22	1.78	0.49
1:A:273:A:O2'	1:A:274:A:H5'	2.13	0.49
1:A:390:C:O3'	16:P:28:ARG:NH2	2.45	0.49
1:A:834:C:H2'	1:A:835:U:H6	1.77	0.49
1:A:868:C:C2'	1:A:869:G:H5'	2.41	0.49
5:E:28:PHE:O	5:E:47:LYS:HA	2.12	0.49
6:F:61:LEU:HD13	6:F:63:TYR:OH	2.12	0.49
6:F:3:ARG:HA	6:F:66:GLU:HA	1.95	0.49
9:I:81:ILE:O	9:I:85:LEU:HB2	2.13	0.49
10:J:49:VAL:O	10:J:60:ARG:CA	2.60	0.49
10:J:9:ARG:CB	10:J:9:ARG:NH1	2.74	0.49
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.13	0.49
18:R:37:VAL:HG22	18:R:78:LEU:HB3	1.95	0.49
19:S:17:GLU:CA	19:S:20:LEU:HG	2.38	0.49
1:A:1184:G:H2'	1:A:1185:G:H8	1.77	0.49
1:A:1208:C:H2'	1:A:1209:C:H6	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:A:H2'	1:A:150:C:C6	2.47	0.49
1:A:19:C:H2'	1:A:20:U:C6	2.48	0.49
1:A:518:C:H2'	1:A:530:G:N3	2.26	0.49
10:J:22:LYS:NZ	10:J:91:PRO:HD3	2.26	0.49
11:K:109:VAL:CG2	18:R:86:VAL:HG22	2.43	0.49
13:M:108:ARG:NH2	13:M:114:ARG:HA	2.28	0.49
23:Y:3:G:O5'	23:Y:3:G:H8	1.95	0.49
1:A:1532:U:H2'	1:A:1533:C:H4'	1.95	0.49
1:A:614:A:C2	1:A:627:G:C2	3.01	0.49
2:B:27:LYS:HD3	2:B:195:ASP:OD2	2.13	0.49
1:A:1113:C:H4'	3:C:14:ILE:HD11	1.94	0.49
5:E:11:ILE:HG12	5:E:33:VAL:HG23	1.94	0.49
9:I:25:LYS:HG2	9:I:60:ASP:OD1	2.13	0.49
13:M:19:LEU:O	13:M:22:ILE:HG13	2.13	0.49
14:N:12:ARG:O	14:N:14:PRO:N	2.45	0.49
17:Q:9:VAL:HG21	17:Q:84:LEU:HD13	1.94	0.49
1:A:1005:A:C2'	1:A:1006:C:H5'	2.42	0.49
2:B:69:LEU:HD23	2:B:69:LEU:C	2.33	0.49
3:C:179:ARG:O	3:C:179:ARG:HG2	2.13	0.49
5:E:144:THR:HG23	5:E:145:LYS:N	2.28	0.49
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.45	0.49
11:K:24:SER:C	11:K:88:GLY:HA3	2.33	0.49
10:J:64:GLU:CB	14:N:59:ALA:HB2	2.38	0.49
1:A:1420:C:H2'	1:A:1421:G:H8	1.78	0.49
1:A:1423:G:O2'	1:A:1424:C:H5'	2.13	0.49
1:A:532:A:H2'	1:A:533:A:H5"	1.94	0.49
1:A:895:G:H2'	1:A:896:C:C6	2.47	0.49
2:B:12:GLU:C	2:B:14:GLY:N	2.66	0.49
2:B:165:VAL:O	2:B:187:LEU:O	2.31	0.49
3:C:132:ARG:HA	3:C:135:LYS:HD2	1.95	0.49
3:C:33:LEU:HD11	14:N:53:LEU:CD2	2.43	0.49
3:C:57:ILE:HG23	3:C:64:VAL:CG1	2.42	0.49
6:F:38:GLU:HB2	6:F:64:GLN:O	2.12	0.49
13:M:110:ARG:HG2	13:M:110:ARG:HH11	1.77	0.49
16:P:20:VAL:HG11	16:P:32:TYR:CB	2.43	0.49
17:Q:74:LEU:O	17:Q:74:LEU:HD22	2.13	0.49
1:A:1394:A:C5	1:A:1501:C:H4'	2.48	0.49
1:A:1488:G:O2'	1:A:1489:G:H5'	2.13	0.49
1:A:279:A:H4'	1:A:280:C:OP2	2.11	0.49
1:A:976:G:N7	1:A:1358:U:C2	2.81	0.49
1:A:991:U:O2'	1:A:992:U:H5'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:SER:O	3:C:164:ARG:O	2.31	0.49
9:I:117:HIS:C	9:I:118:LYS:HG3	2.33	0.49
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.95	0.49
13:M:37:THR:O	13:M:37:THR:HG22	2.13	0.49
19:S:16:LEU:O	19:S:19:VAL:HG12	2.13	0.49
20:T:100:ILE:O	20:T:101:GLY:C	2.51	0.49
1:A:1141:C:H2'	1:A:1142:G:C8	2.46	0.48
1:A:634:C:O2'	1:A:635:G:H5'	2.13	0.48
1:A:791:G:C2'	1:A:792:A:C5'	2.91	0.48
2:B:144:ARG:HG3	2:B:145:LEU:H	1.78	0.48
2:B:71:VAL:HG12	2:B:170:GLU:HG2	1.95	0.48
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.94	0.48
3:C:21:ARG:NH1	3:C:21:ARG:HG2	2.26	0.48
4:D:148:VAL:CG1	4:D:158:ILE:HD13	2.43	0.48
10:J:8:LEU:HD23	10:J:96:ILE:HG23	1.95	0.48
14:N:11:LYS:O	14:N:11:LYS:HG3	2.12	0.48
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.94	0.48
1:A:1060:C:H2'	1:A:1061:G:H8	1.77	0.48
1:A:476:G:C2	1:A:477:G:C8	3.01	0.48
2:B:118:LEU:HB2	2:B:142:LEU:HD21	1.95	0.48
2:B:10:LEU:HG	2:B:48:MET:HE1	1.96	0.48
3:C:102:ASN:N	3:C:102:ASN:ND2	2.61	0.48
3:C:11:ARG:NH1	3:C:177:THR:O	2.46	0.48
3:C:58:GLU:H	3:C:65:ALA:HB3	1.78	0.48
4:D:25:ARG:C	4:D:27:TYR:N	2.66	0.48
5:E:45:PHE:CD2	5:E:47:LYS:HE3	2.48	0.48
5:E:40:ARG:NH1	5:E:68:GLU:OE1	2.46	0.48
1:A:1128:C:H5'	9:I:16:ARG:HH12	1.78	0.48
10:J:8:LEU:HB3	10:J:16:LEU:HD22	1.94	0.48
15:O:81:LEU:CD2	15:O:85:LEU:HD12	2.43	0.48
18:R:87:ARG:O	18:R:88:LYS:HB2	2.13	0.48
1:A:195:A:H4'	20:T:68:LYS:HE2	1.95	0.48
21:U:2:GLY:O	21:U:4:GLY:N	2.46	0.48
1:A:613:C:O2'	1:A:614:A:H5'	2.13	0.48
1:A:939:G:H5"	7:G:102:ARG:CZ	2.43	0.48
1:A:966:G:OP1	1:A:966:G:H8	1.95	0.48
4:D:189:PRO:HB2	4:D:194:LEU:HD21	1.95	0.48
5:E:144:THR:HG23	5:E:146:ALA:H	1.78	0.48
6:F:52:ILE:O	6:F:53:ALA:HB3	2.14	0.48
1:A:972:C:OP1	10:J:57:LYS:HE2	2.14	0.48
10:J:9:ARG:HH11	10:J:9:ARG:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:11:LYS:O	11:K:12:ARG:HB2	2.13	0.48
15:O:60:VAL:O	15:O:64:ARG:HG2	2.13	0.48
1:A:376:G:OP2	16:P:67:THR:HG21	2.13	0.48
1:A:1128:C:H4'	9:I:16:ARG:HH12	1.77	0.48
1:A:1285:A:OP1	1:A:1285:A:H8	1.96	0.48
1:A:1539:C:H5	7:G:81:GLY:HA2	1.78	0.48
1:A:346:G:C2'	1:A:347:G:H5'	2.43	0.48
1:A:987:G:H2'	1:A:988:G:C8	2.47	0.48
2:B:134:GLU:HB3	2:B:138:LEU:HD12	1.95	0.48
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.94	0.48
9:I:30:GLY:O	9:I:31:GLN:O	2.32	0.48
17:Q:7:THR:O	17:Q:23:VAL:HG13	2.13	0.48
1:A:1327:C:O2'	1:A:1328:C:H5'	2.13	0.48
1:A:1347:G:C2'	1:A:1348:U:OP2	2.62	0.48
1:A:335:C:H2'	1:A:336:C:C6	2.48	0.48
1:A:628:G:H2'	1:A:629:G:C8	2.48	0.48
1:A:838:G:N2	1:A:849:C:C2	2.81	0.48
1:A:947:G:H2'	1:A:948:C:O4'	2.13	0.48
6:F:40:VAL:CG2	6:F:41:GLU:N	2.76	0.48
7:G:145:ALA:O	7:G:147:ALA:N	2.42	0.48
7:G:93:PRO:HG2	7:G:94:ARG:H	1.77	0.48
13:M:102:ARG:HG3	13:M:102:ARG:O	2.13	0.48
13:M:4:ILE:CG2	13:M:5:ALA:N	2.70	0.48
14:N:12:ARG:O	14:N:14:PRO:CD	2.61	0.48
17:Q:104:LYS:O	17:Q:105:ALA:OXT	2.31	0.48
17:Q:68:ARG:NH1	17:Q:68:ARG:CG	2.74	0.48
1:A:1499:A:H1'	1:A:1520:G:H5'	1.95	0.48
1:A:1521:G:H2'	1:A:1522:U:C6	2.49	0.48
1:A:342:C:C2'	1:A:343:U:H5'	2.43	0.48
1:A:824:C:H2'	1:A:825:G:H8	1.78	0.48
3:C:113:ALA:HB3	3:C:114:PRO:HD3	1.94	0.48
3:C:52:LEU:HD21	3:C:118:GLN:NE2	2.23	0.48
3:C:70:VAL:CG1	3:C:71:ALA:N	2.75	0.48
5:E:10:MET:SD	5:E:13:ILE:HG23	2.54	0.48
5:E:51:VAL:HB	5:E:52:PRO:CD	2.39	0.48
5:E:79:GLU:HG3	5:E:93:PRO:CD	2.42	0.48
1:A:711:G:P	6:F:54:LYS:HZ3	2.36	0.48
9:I:13:ALA:CB	9:I:67:GLY:O	2.61	0.48
14:N:24:CYS:HB2	14:N:29:ARG:HB3	1.94	0.48
1:A:1343:G:H2'	1:A:1344:C:H6	1.75	0.48
1:A:202:U:C5'	1:A:203:U:OP2	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:A:C2'	1:A:394:G:H5'	2.43	0.48
1:A:420:U:O2'	1:A:421:U:H5"	2.13	0.48
1:A:971:G:OP1	1:A:972:C:H5"	2.14	0.48
2:B:162:ILE:HD12	2:B:177:ALA:HB2	1.96	0.48
2:B:52:GLU:CD	2:B:56:ARG:HH21	2.17	0.48
5:E:81:GLU:HG2	5:E:88:LYS:HE2	1.95	0.48
9:I:118:LYS:O	9:I:119:ALA:HB3	2.13	0.48
13:M:49:THR:HB	13:M:52:GLU:CG	2.33	0.48
3:C:33:LEU:HD11	14:N:53:LEU:HD23	1.95	0.48
1:A:192:U:C1'	20:T:103:GLY:HA2	2.43	0.48
1:A:530:G:O6	23:Y:3:G:H1'	2.14	0.48
1:A:151:A:H2'	1:A:152:A:O4'	2.13	0.48
1:A:750:G:N3	15:O:23:GLY:HA3	2.29	0.48
1:A:942:G:H2'	1:A:943:U:H6	1.78	0.48
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.95	0.48
4:D:64:LEU:HD11	4:D:97:LEU:HD11	1.96	0.48
6:F:53:ALA:O	6:F:55:ASP:N	2.46	0.48
7:G:113:GLU:CG	7:G:119:ARG:HG2	2.37	0.48
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.48	0.48
12:L:46:LYS:HD2	12:L:47:LYS:HG3	1.96	0.48
17:Q:45:HIS:HB3	17:Q:72:ARG:HG2	1.95	0.48
20:T:10:LEU:CD1	20:T:12:ALA:HB3	2.42	0.48
1:A:1032:G:H2'	1:A:1033:G:C8	2.48	0.48
1:A:1300:G:O2'	1:A:1301:U:P	2.71	0.48
1:A:1501:C:OP2	1:A:1504:G:H2'	2.14	0.48
1:A:180:U:H2'	1:A:181:G:H5'	1.96	0.48
1:A:50:A:N6	1:A:361:G:H4'	2.29	0.48
3:C:106:VAL:HG11	3:C:112:SER:OG	2.14	0.48
5:E:31:LEU:HD22	5:E:43:LEU:CD2	2.43	0.48
10:J:23:ILE:N	10:J:23:ILE:HD12	2.28	0.48
14:N:23:ARG:HG2	14:N:23:ARG:HH11	1.79	0.48
19:S:14:HIS:O	19:S:18:LYS:HE3	2.14	0.48
1:A:1320:C:N4	19:S:37:ARG:NH1	2.61	0.48
1:A:1260:C:O5'	1:A:1284:C:H4'	2.13	0.48
1:A:1288:A:H1'	1:A:1352:C:HO2'	1.78	0.48
1:A:1399:C:C2	1:A:1502:A:N6	2.82	0.48
1:A:423:G:H2'	1:A:424:G:O4'	2.14	0.48
1:A:867:G:O2'	1:A:868:C:H5'	2.13	0.48
3:C:19:GLU:HG2	3:C:54:ARG:HE	1.79	0.48
8:H:82:HIS:CD2	8:H:83:ILE:H	2.31	0.48
9:I:103:THR:HG22	9:I:104:ARG:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:22:LYS:HE2	10:J:90:LEU:H	1.77	0.48
13:M:5:ALA:HB3	13:M:8:GLU:HG3	1.94	0.48
20:T:43:LEU:HD13	20:T:51:GLU:HG3	1.95	0.48
20:T:94:ALA:O	20:T:95:ALA:CB	2.61	0.48
1:A:1196:U:H4'	1:A:1197:G:OP2	2.13	0.47
1:A:1380:U:O2'	1:A:1381:U:OP2	2.27	0.47
1:A:408:A:O2'	1:A:409:G:H5'	2.14	0.47
2:B:124:SER:OG	2:B:126:GLU:HG3	2.14	0.47
4:D:35:ARG:O	4:D:36:ARG:HG3	2.15	0.47
7:G:116:ALA:HA	7:G:119:ARG:CZ	2.43	0.47
15:O:88:ARG:CB	15:O:88:ARG:HH11	2.25	0.47
17:Q:5:VAL:HA	17:Q:59:ILE:O	2.13	0.47
1:A:1030:C:H2'	1:A:1030(A):G:H8	1.78	0.47
1:A:343:U:H2'	1:A:345:C:C5	2.48	0.47
2:B:35:GLU:HA	2:B:39:ILE:O	2.14	0.47
4:D:31:CYS:C	4:D:33:MET:H	2.17	0.47
4:D:62:GLN:HE22	4:D:65:ARG:HH11	1.58	0.47
5:E:45:PHE:CE2	5:E:47:LYS:HE3	2.49	0.47
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.48	0.47
1:A:1280:A:H5'	10:J:40:LEU:HD22	1.95	0.47
1:A:718:G:H5'	11:K:117:ASN:ND2	2.29	0.47
12:L:83:VAL:HG12	12:L:84:LEU:N	2.28	0.47
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.13	0.47
14:N:5:ALA:O	14:N:8:GLU:HG2	2.14	0.47
17:Q:45:HIS:NE2	17:Q:47:PRO:HG3	2.28	0.47
19:S:80:TYR:CG	19:S:81:ARG:N	2.82	0.47
1:A:1229:A:H2'	1:A:1230:C:C6	2.49	0.47
1:A:1298:C:H2'	7:G:114:ARG:HH12	1.80	0.47
1:A:251:G:H4'	1:A:252:U:O5'	2.14	0.47
2:B:132:LYS:O	2:B:135:GLN:HB2	2.15	0.47
2:B:80:ILE:N	2:B:80:ILE:HD12	2.22	0.47
3:C:178:LEU:O	3:C:179:ARG:HB2	2.15	0.47
3:C:195:VAL:O	3:C:196:LEU:HD22	2.13	0.47
4:D:173:TRP:O	4:D:186:LEU:HB2	2.14	0.47
4:D:33:MET:O	4:D:37:PRO:HG3	2.14	0.47
6:F:99:ALA:O	6:F:100:ASN:HB3	2.14	0.47
10:J:22:LYS:HE3	10:J:90:LEU:HB2	1.95	0.47
10:J:75:ILE:O	10:J:76:ASN:HB2	2.15	0.47
11:K:69:ALA:CB	11:K:101:SER:HB2	2.45	0.47
12:L:41:ARG:HH12	12:L:57:LYS:NZ	2.12	0.47
13:M:94:ARG:NH1	13:M:94:ARG:HG3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:1:MET:HE3	16:P:3:LYS:HD2	1.95	0.47
1:A:1049:U:OP1	14:N:3:ARG:HG3	2.14	0.47
1:A:197:A:N1	1:A:220:G:O2'	2.46	0.47
2:B:62:ALA:C	2:B:64:ARG:H	2.16	0.47
3:C:42:LEU:O	3:C:46:GLU:HG2	2.14	0.47
16:P:67:THR:N	16:P:70:ALA:HB3	2.30	0.47
1:A:1129:C:O2'	1:A:1130:A:P	2.73	0.47
1:A:1241:G:H2'	1:A:1242:C:H6	1.78	0.47
1:A:1312:G:N7	19:S:3:ARG:O	2.47	0.47
1:A:403:C:O2'	1:A:404:U:H5'	2.13	0.47
1:A:925:G:C2	1:A:927:G:C8	3.03	0.47
1:A:948:C:O2'	1:A:949:A:H5'	2.15	0.47
1:A:1101:A:C8	2:B:172:ILE:HD13	2.50	0.47
2:B:23:ARG:O	2:B:24:TRP:O	2.32	0.47
4:D:28:SER:C	4:D:30:LYS:H	2.17	0.47
11:K:13:GLN:HA	11:K:75:TYR:O	2.14	0.47
15:O:17:ARG:NH1	15:O:17:ARG:CG	2.73	0.47
21:U:12:LYS:HG2	21:U:22:ARG:HB3	1.96	0.47
1:A:1044:A:C2'	1:A:1045:C:H5'	2.45	0.47
1:A:1195:C:H3'	1:A:1196:U:H5'	1.96	0.47
1:A:538:G:H2'	1:A:539:A:H8	1.80	0.47
2:B:162:ILE:CG2	2:B:164:VAL:HG23	2.44	0.47
3:C:107:GLN:H	3:C:107:GLN:CD	2.17	0.47
3:C:70:VAL:C	3:C:106:VAL:HG23	2.34	0.47
4:D:35:ARG:O	4:D:35:ARG:HG3	2.14	0.47
7:G:146:GLU:HG2	7:G:149:ARG:NH2	2.23	0.47
9:I:118:LYS:NZ	9:I:118:LYS:CB	2.77	0.47
10:J:19:SER:CA	10:J:22:LYS:HZ3	2.24	0.47
13:M:22:ILE:HB	13:M:25:ILE:HB	1.97	0.47
16:P:28:ARG:HG3	16:P:29:ASP:N	2.29	0.47
6:F:97:PHE:HB2	18:R:32:ARG:NH2	2.29	0.47
19:S:40:ILE:HG21	19:S:62:ILE:CD1	2.44	0.47
1:A:1054:C:H4'	1:A:1055:A:C5'	2.45	0.47
1:A:1248:A:H1'	9:I:70:LYS:NZ	2.30	0.47
1:A:409:G:N1	1:A:434:U:C5	2.75	0.47
1:A:570:G:H2'	1:A:571:U:C6	2.49	0.47
1:A:959:A:H5"	1:A:960:U:OP2	2.14	0.47
2:B:178:ARG:HH22	8:H:74:PRO:HB3	1.79	0.47
2:B:52:GLU:HG2	2:B:56:ARG:NH2	2.29	0.47
3:C:129:ALA:HB3	3:C:132:ARG:NH1	2.28	0.47
10:J:4:ILE:HG23	10:J:100:THR:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.95	0.47
1:A:1036:G:H2'	1:A:1037:C:C6	2.50	0.47
1:A:1328:C:H2'	1:A:1329:A:O4'	2.14	0.47
1:A:1503:A:H4'	1:A:1504:G:OP1	2.15	0.47
1:A:828:A:H2'	1:A:829:G:O4'	2.15	0.47
2:B:121:LEU:HB3	2:B:127:ILE:CG2	2.45	0.47
3:C:107:GLN:O	3:C:108:ASN:HB3	2.15	0.47
4:D:146:ILE:N	4:D:146:ILE:CD1	2.78	0.47
5:E:102:ALA:HB1	5:E:120:THR:HG21	1.96	0.47
5:E:51:VAL:CB	5:E:52:PRO:HD3	2.38	0.47
9:I:43:ALA:H	9:I:74:ILE:HD13	1.80	0.47
9:I:46:ALA:HB1	9:I:77:ILE:CG2	2.45	0.47
1:A:1228:C:OP1	13:M:115:LYS:HD3	2.14	0.47
13:M:5:ALA:HB3	13:M:8:GLU:CG	2.45	0.47
14:N:29:ARG:HG2	14:N:40:CYS:HB2	1.96	0.47
21:U:2:GLY:C	21:U:4:GLY:H	2.17	0.47
1:A:1305:G:OP1	21:U:2:GLY:N	2.48	0.47
1:A:1460:A:H2'	1:A:1461:G:O4'	2.15	0.47
1:A:342:C:O2'	1:A:343:U:H5'	2.15	0.47
1:A:627:G:H2'	1:A:628:G:H8	1.80	0.47
1:A:731:G:OP1	1:A:766:A:H1'	2.15	0.47
1:A:76:C:O2'	1:A:77:G:H5'	2.14	0.47
2:B:219:VAL:O	2:B:223:ILE:HG13	2.15	0.47
3:C:83:ARG:C	3:C:85:ARG:N	2.68	0.47
4:D:162:LEU:HD22	4:D:178:VAL:HG13	1.96	0.47
7:G:79:ARG:HG2	7:G:84:ASN:OD1	2.14	0.47
16:P:67:THR:HG22	16:P:69:THR:N	2.30	0.47
17:Q:12:SER:HB3	17:Q:20:THR:HB	1.95	0.47
18:R:28:GLU:OE1	18:R:28:GLU:N	2.48	0.47
20:T:57:ARG:NH1	20:T:57:ARG:HB2	2.18	0.47
1:A:1049:U:H1'	1:A:1201:A:N7	2.30	0.47
1:A:1353:G:H2'	1:A:1354:C:H6	1.80	0.47
1:A:412:A:H1'	1:A:413:G:C2'	2.41	0.47
4:D:8:VAL:HG11	4:D:21:LEU:CB	2.44	0.47
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.79	0.47
9:I:118:LYS:NZ	9:I:118:LYS:HB2	2.29	0.47
13:M:65:LYS:HD3	13:M:69:GLU:HG2	1.96	0.47
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.50	0.47
1:A:1271:G:H2'	1:A:1272:G:C8	2.50	0.47
1:A:1314:C:OP2	19:S:6:LYS:CD	2.62	0.47
1:A:1352:C:H2'	1:A:1353:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:G:H2'	1:A:256:U:C6	2.50	0.47
1:A:255:G:O6	1:A:266:G:O6	2.32	0.47
1:A:287:U:O2'	1:A:288:A:H5'	2.14	0.47
1:A:338:A:H2'	1:A:339:C:C6	2.49	0.47
1:A:474:G:H4'	16:P:81:ARG:CZ	2.46	0.47
1:A:517:G:N1	1:A:533:A:OP2	2.42	0.47
1:A:755:G:OP2	15:O:65:ARG:HG2	2.14	0.47
1:A:834:C:H2'	1:A:835:U:C6	2.50	0.47
2:B:19:HIS:ND1	2:B:204:ASN:HB3	2.28	0.47
3:C:132:ARG:HB3	3:C:132:ARG:HH11	1.79	0.47
3:C:40:ARG:HG2	3:C:55:VAL:HG11	1.97	0.47
5:E:152:ARG:O	8:H:64:LYS:NZ	2.48	0.47
13:M:9:ILE:HD12	13:M:9:ILE:H	1.78	0.47
18:R:38:GLU:HA	18:R:41:LYS:CE	2.31	0.47
1:A:1206:G:C6	1:A:1207:G:C5	3.04	0.46
1:A:1273:G:H2'	1:A:1274:G:C8	2.51	0.46
1:A:1413:A:H2	1:A:1487:G:H22	1.62	0.46
1:A:663:A:O2'	1:A:664:G:H5'	2.15	0.46
6:F:86:ARG:O	6:F:87:ARG:HG2	2.15	0.46
6:F:91:VAL:HG12	6:F:92:LYS:O	2.14	0.46
7:G:18:TYR:OH	7:G:58:PRO:HG2	2.16	0.46
1:A:1165:C:C2'	1:A:1166:G:H5'	2.45	0.46
1:A:1281:U:H4'	1:A:1282:C:OP2	2.14	0.46
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.50	0.46
1:A:946:A:H2'	1:A:947:G:H8	1.79	0.46
1:A:961:U:H2'	1:A:962:C:H5'	1.96	0.46
2:B:17:PHE:HB2	2:B:41:ILE:HG23	1.97	0.46
1:A:1111:A:N6	3:C:177:THR:HA	2.29	0.46
3:C:91:LEU:HD23	3:C:92:ALA:N	2.30	0.46
9:I:9:ARG:HD3	9:I:14:VAL:HG22	1.97	0.46
16:P:19:ILE:HG22	16:P:36:ILE:CG1	2.40	0.46
1:A:1167:A:H2'	1:A:1168:A:C8	2.50	0.46
1:A:26:A:N6	1:A:558:G:H1'	2.31	0.46
1:A:560:U:H5'	1:A:566:G:N2	2.30	0.46
2:B:118:LEU:O	2:B:120:ALA:N	2.48	0.46
5:E:102:ALA:CB	5:E:120:THR:HG21	2.45	0.46
2:B:179:LYS:HA	8:H:72:PRO:HD3	1.97	0.46
9:I:58:ARG:HG3	9:I:58:ARG:HH11	1.80	0.46
16:P:19:ILE:CG2	16:P:36:ILE:HG13	2.41	0.46
19:S:19:VAL:HG13	19:S:20:LEU:N	2.31	0.46
1:A:1149:C:H2'	1:A:1150:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1263:C:H2'	1:A:1264:C:H6	1.80	0.46
1:A:192:U:O4'	20:T:103:GLY:HA2	2.15	0.46
1:A:883:C:O2'	1:A:884:U:H5'	2.15	0.46
5:E:36:ASP:O	5:E:37:ARG:HB2	2.16	0.46
5:E:64:ARG:O	5:E:65:ASN:HB3	2.15	0.46
5:E:72:GLN:O	5:E:73:ASN:HB3	2.15	0.46
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.51	0.46
9:I:55:ALA:O	9:I:56:LEU:HB3	2.15	0.46
10:J:23:ILE:CG2	10:J:72:VAL:HG11	2.46	0.46
15:O:70:LEU:HD12	15:O:78:TYR:N	2.30	0.46
19:S:80:TYR:CD2	19:S:81:ARG:N	2.84	0.46
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.49	0.46
1:A:489:C:H2'	1:A:490:G:H8	1.79	0.46
2:B:86:GLU:C	2:B:88:ALA:N	2.66	0.46
3:C:2:GLY:C	3:C:3:ASN:HD22	2.15	0.46
3:C:82:GLU:HG3	3:C:82:GLU:O	2.16	0.46
5:E:122:GLU:OE1	5:E:131:ILE:HG13	2.16	0.46
14:N:34:TYR:HD1	14:N:34:TYR:H	1.62	0.46
16:P:67:THR:HB	16:P:70:ALA:HB2	1.98	0.46
18:R:53:ARG:HH11	18:R:59:SER:HA	1.80	0.46
18:R:53:ARG:HA	18:R:56:THR:OG1	2.14	0.46
1:A:1279:A:O2'	1:A:1282:C:N4	2.49	0.46
1:A:1306:A:N6	1:A:1331:G:H1'	2.30	0.46
1:A:1401:G:C2	1:A:1402:C:H1'	2.50	0.46
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.69	0.46
1:A:1111:A:N1	3:C:177:THR:HB	2.30	0.46
3:C:38:ARG:HH11	3:C:38:ARG:HG3	1.80	0.46
3:C:79:ARG:C	3:C:81:GLY:H	2.18	0.46
3:C:35:GLU:CG	3:C:95:THR:HG21	2.46	0.46
4:D:31:CYS:O	4:D:32:ALA:HB3	2.15	0.46
6:F:32:ASN:N	6:F:32:ASN:ND2	2.62	0.46
7:G:46:ALA:O	7:G:50:ILE:HG13	2.16	0.46
8:H:111:ILE:O	8:H:134:ILE:HB	2.16	0.46
9:I:50:LEU:HG	9:I:81:ILE:HG21	1.98	0.46
17:Q:48:GLU:C	17:Q:50:LYS:N	2.67	0.46
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.97	0.46
19:S:41:VAL:HB	19:S:42:PRO:HD2	1.97	0.46
1:A:1061:G:C6	1:A:1062:U:N3	2.84	0.46
1:A:1091:U:O2	1:A:1093:A:C8	2.68	0.46
1:A:620:C:H2'	1:A:621:A:O4'	2.16	0.46
1:A:629:G:O2'	1:A:630:G:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:G:C6	1:A:851:G:C6	3.04	0.46
2:B:118:LEU:HB3	2:B:142:LEU:CD1	2.45	0.46
2:B:157:ARG:HH11	2:B:157:ARG:HG3	1.80	0.46
2:B:178:ARG:HH21	8:H:68:ARG:NH2	2.13	0.46
3:C:35:GLU:OE1	3:C:95:THR:HG21	2.16	0.46
4:D:30:LYS:C	4:D:32:ALA:H	2.19	0.46
9:I:10:ARG:HG2	9:I:75:ASP:CB	2.46	0.46
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.69	0.46
3:C:13:GLY:CA	14:N:57:ARG:HH21	2.24	0.46
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.97	0.46
18:R:39:VAL:CG1	18:R:40:LEU:N	2.78	0.46
1:A:1044:A:H2'	1:A:1045:C:C5'	2.46	0.46
1:A:1054:C:H4'	1:A:1055:A:O5'	2.15	0.46
1:A:123:C:OP1	1:A:312:C:H5'	2.15	0.46
1:A:528:C:H5'	1:A:535:A:C6	2.50	0.46
1:A:939:G:H2'	1:A:940:C:C6	2.51	0.46
4:D:103:ASN:O	4:D:106:TYR:HB3	2.16	0.46
4:D:70:ILE:HG22	4:D:71:SER:H	1.81	0.46
7:G:6:ARG:O	7:G:7:ALA:C	2.54	0.46
9:I:114:TYR:CE1	10:J:59:SER:O	2.69	0.46
12:L:60:LEU:CD2	12:L:66:VAL:HG22	2.45	0.46
19:S:8:GLY:O	19:S:9:VAL:C	2.53	0.46
1:A:1018:C:H6	1:A:1018:C:O5'	1.98	0.46
1:A:1251:A:H2'	1:A:1252:A:C8	2.51	0.46
1:A:22:G:H4'	1:A:885:G:C8	2.51	0.46
1:A:952:U:O2'	1:A:953:G:H5'	2.16	0.46
3:C:79:ARG:HE	3:C:82:GLU:CG	2.28	0.46
3:C:86:VAL:O	3:C:90:GLU:HG2	2.16	0.46
6:F:19:LEU:HD23	6:F:20:ALA:N	2.31	0.46
10:J:4:ILE:O	10:J:6:ILE:HG12	2.16	0.46
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.98	0.46
13:M:5:ALA:O	13:M:7:VAL:N	2.48	0.46
17:Q:67:LYS:HG2	17:Q:68:ARG:N	2.30	0.46
21:U:9:ARG:CZ	21:U:22:ARG:HA	2.45	0.46
1:A:1451:A:O2'	1:A:1452:C:OP1	2.28	0.46
1:A:791:G:C2'	1:A:792:A:H5"	2.46	0.46
1:A:987:G:H2'	1:A:988:G:H8	1.80	0.46
2:B:98:LEU:N	2:B:98:LEU:CD2	2.79	0.46
2:B:98:LEU:N	2:B:98:LEU:HD22	2.30	0.46
3:C:90:GLU:HA	3:C:93:LYS:HG3	1.97	0.46
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18:TYR:N	7:G:18:TYR:CD1	2.84	0.46
7:G:54:THR:CG2	7:G:55:GLY:N	2.78	0.46
12:L:41:ARG:HB3	12:L:41:ARG:HH11	1.81	0.46
20:T:14:LYS:O	20:T:18:GLN:HG3	2.15	0.46
1:A:327:A:O3'	1:A:328:C:H4'	2.16	0.45
1:A:807:A:H2'	1:A:808:C:H6	1.81	0.45
3:C:115:LEU:O	3:C:118:GLN:N	2.49	0.45
5:E:24:ARG:HG2	5:E:24:ARG:NH1	2.26	0.45
9:I:49:PRO:HB3	9:I:82:ALA:HB2	1.97	0.45
10:J:6:ILE:HG13	10:J:72:VAL:HB	1.97	0.45
13:M:22:ILE:CD1	13:M:25:ILE:HD12	2.46	0.45
17:Q:98:LEU:H	17:Q:98:LEU:CD2	2.27	0.45
1:A:109:A:H2'	1:A:326:G:N2	2.31	0.45
1:A:343:U:H2'	1:A:345:C:C4	2.51	0.45
1:A:375:U:O3'	16:P:6:LEU:HB2	2.16	0.45
1:A:922:G:N3	1:A:1398:A:H2	2.14	0.45
2:B:112:VAL:O	2:B:116:GLU:HG3	2.17	0.45
3:C:115:LEU:HD23	3:C:118:GLN:OE1	2.16	0.45
6:F:47:ARG:HA	6:F:57:GLN:HG2	1.97	0.45
2:B:178:ARG:NH2	8:H:68:ARG:NH2	2.63	0.45
12:L:10:LEU:HB3	17:Q:32:TYR:CE1	2.51	0.45
17:Q:74:LEU:O	17:Q:75:ARG:CB	2.61	0.45
18:R:45:SER:O	18:R:47:THR:O	2.35	0.45
1:A:1025:U:H4'	1:A:1025:U:OP1	2.17	0.45
1:A:1030:C:H2'	1:A:1030(A):G:C8	2.51	0.45
1:A:1108:G:H4'	1:A:1191:A:O4'	2.16	0.45
1:A:338:A:H2	1:A:351:G:H22	1.63	0.45
1:A:389:A:H2'	1:A:390:C:O4'	2.15	0.45
1:A:686:U:O2'	1:A:687:A:C8	2.52	0.45
2:B:144:ARG:HA	2:B:147:LYS:HD2	1.97	0.45
2:B:206:ASP:O	2:B:207:ALA:CB	2.64	0.45
5:E:75:THR:HG23	5:E:76:ILE:N	2.31	0.45
6:F:22:GLU:O	6:F:26:ILE:HG13	2.17	0.45
12:L:113:ARG:NH1	12:L:116:SER:H	2.14	0.45
12:L:86:ARG:HG3	12:L:86:ARG:NH1	2.29	0.45
13:M:63:THR:HG23	13:M:64:TRP:CG	2.51	0.45
16:P:82:GLN:O	16:P:84:ALA:N	2.49	0.45
1:A:1520:G:O2'	1:A:1521:G:H5'	2.16	0.45
1:A:879:C:O2'	1:A:880:C:H5'	2.17	0.45
2:B:102:LEU:CD1	2:B:102:LEU:N	2.79	0.45
2:B:77:ALA:HA	2:B:80:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:LYS:HE3	3:C:203:PHE:CE2	2.52	0.45
7:G:120:ILE:N	7:G:120:ILE:HD12	2.30	0.45
7:G:31:MET:SD	7:G:34:GLY:HA2	2.57	0.45
11:K:51:LYS:O	11:K:55:LYS:HE2	2.16	0.45
13:M:5:ALA:O	13:M:6:GLY:C	2.53	0.45
13:M:9:ILE:N	13:M:9:ILE:CD1	2.79	0.45
1:A:1063:C:H2'	1:A:1064:G:C8	2.52	0.45
1:A:17:U:H1'	1:A:1080:A:N3	2.31	0.45
1:A:1476:G:O2'	1:A:1477:C:H5'	2.16	0.45
1:A:102:G:O2'	1:A:151:A:N3	2.43	0.45
1:A:503:C:H2'	1:A:504:C:H6	1.81	0.45
1:A:707:C:H2'	1:A:708:C:C6	2.51	0.45
2:B:30:ARG:HG3	2:B:31:TYR:CD2	2.52	0.45
2:B:7:VAL:C	2:B:8:LYS:HG3	2.36	0.45
3:C:77:ILE:HA	3:C:84:ILE:HB	1.98	0.45
3:C:79:ARG:NH2	3:C:82:GLU:HG2	2.24	0.45
4:D:173:TRP:HB2	4:D:187:ARG:O	2.17	0.45
4:D:30:LYS:O	4:D:32:ALA:N	2.50	0.45
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.98	0.45
9:I:9:ARG:HG2	9:I:14:VAL:HG22	1.96	0.45
10:J:60:ARG:O	10:J:61:GLU:HB3	2.17	0.45
11:K:50:TYR:HB3	11:K:54:ARG:HB2	1.98	0.45
14:N:37:PHE:CZ	14:N:56:VAL:HG21	2.52	0.45
19:S:15:LEU:O	19:S:16:LEU:C	2.55	0.45
20:T:82:SER:O	20:T:86:ARG:HB2	2.16	0.45
1:A:1168:A:H2'	1:A:1169:A:C8	2.52	0.45
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.38	0.45
1:A:417:C:H3'	1:A:418:C:C5	2.52	0.45
2:B:137:ARG:CB	2:B:137:ARG:NH1	2.79	0.45
3:C:123:GLN:NE2	3:C:140:ARG:HH22	2.14	0.45
3:C:19:GLU:O	3:C:40:ARG:NH2	2.50	0.45
3:C:90:GLU:O	3:C:93:LYS:HB2	2.15	0.45
6:F:53:ALA:C	6:F:55:ASP:N	2.70	0.45
6:F:12:PRO:HG3	6:F:55:ASP:OD1	2.16	0.45
8:H:38:ILE:N	8:H:38:ILE:HD12	2.28	0.45
1:A:1349:A:OP2	9:I:118:LYS:NZ	2.49	0.45
9:I:127:LYS:CD	9:I:127:LYS:H	2.17	0.45
1:A:1152:A:C5'	10:J:13:HIS:HB2	2.46	0.45
16:P:74:LEU:HB3	16:P:79:VAL:HG21	1.97	0.45
17:Q:44:ALA:HB2	17:Q:59:ILE:HD12	1.99	0.45
18:R:53:ARG:NH1	18:R:60:ALA:N	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:108:ILE:CD1	18:R:88:LYS:HB3	2.46	0.45
1:A:1320:C:C2	19:S:72:GLY:HA3	2.52	0.45
1:A:1094:G:OP2	1:A:1095:U:C5	2.70	0.45
1:A:862:C:O2'	1:A:863:U:H5'	2.17	0.45
2:B:17:PHE:O	2:B:18:GLY:O	2.35	0.45
3:C:11:ARG:O	3:C:14:ILE:O	2.34	0.45
3:C:167:TRP:O	3:C:168:ALA:HB3	2.15	0.45
3:C:53:ALA:O	3:C:54:ARG:HB2	2.17	0.45
4:D:35:ARG:O	4:D:36:ARG:HB2	2.16	0.45
12:L:102:ARG:HB2	12:L:120:TYR:HA	1.99	0.45
12:L:119:LYS:O	12:L:120:TYR:HB2	2.17	0.45
12:L:33:ARG:HA	12:L:33:ARG:HE	1.81	0.45
1:A:1206:G:O2'	1:A:1207:G:H5'	2.17	0.45
1:A:265:G:H2'	1:A:267:C:H5	1.82	0.45
1:A:514:C:O2'	1:A:515:G:H5'	2.17	0.45
1:A:782:A:H2'	1:A:783:C:O4'	2.17	0.45
3:C:134:ILE:HG22	3:C:168:ALA:CB	2.47	0.45
3:C:138:VAL:O	3:C:142:MET:HB2	2.17	0.45
3:C:90:GLU:HA	3:C:93:LYS:HB2	1.98	0.45
4:D:121:VAL:O	4:D:134:ASP:HA	2.17	0.45
8:H:117:GLY:O	8:H:119:LEU:HG	2.17	0.45
13:M:110:ARG:HH11	13:M:110:ARG:CG	2.29	0.45
14:N:57:ARG:HG2	14:N:58:LYS:N	2.24	0.45
17:Q:26:GLN:HG2	17:Q:37:LYS:HG2	1.98	0.45
1:A:1003(A):G:C6	1:A:1004:A:H1'	2.52	0.45
1:A:1300:G:HO2'	1:A:1301:U:H6	1.63	0.45
1:A:1508:G:O2'	1:A:1509:C:H5'	2.17	0.45
1:A:129(A):G:O2'	1:A:190(E):U:C6	2.68	0.45
1:A:838:G:N2	1:A:848:C:O2	2.43	0.45
2:B:144:ARG:HG3	2:B:145:LEU:N	2.31	0.45
2:B:15:VAL:HG21	2:B:209:ARG:HG3	1.99	0.45
10:J:53:PRO:O	10:J:54:PHE:O	2.35	0.45
10:J:47:PHE:CZ	14:N:37:PHE:HE1	2.34	0.45
16:P:51:VAL:HG11	16:P:74:LEU:HD23	1.99	0.45
1:A:1309:G:O2'	1:A:1310:G:H5'	2.17	0.45
1:A:1342:C:O2'	1:A:1343:G:H5'	2.17	0.45
1:A:1428:A:H2'	1:A:1429:C:C6	2.51	0.45
1:A:167:G:O2'	1:A:168:G:H5'	2.17	0.45
1:A:892:A:C2	1:A:907:A:C4	3.05	0.45
1:A:933:G:O6	7:G:3:ARG:NH2	2.50	0.45
3:C:52:LEU:HG	3:C:52:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:ALA:HA	4:D:161:ASN:HD22	1.81	0.45
4:D:58:LEU:HD22	4:D:58:LEU:O	2.17	0.45
8:H:83:ILE:HA	8:H:136:GLU:O	2.17	0.45
10:J:6:ILE:HD11	10:J:72:VAL:CG1	2.47	0.45
11:K:57:THR:OG1	11:K:58:PRO:HD2	2.16	0.45
14:N:9:LYS:HD3	14:N:10:ALA:CA	2.46	0.45
1:A:1060:C:H2'	1:A:1061:G:C8	2.52	0.44
1:A:1154:G:O2'	1:A:1155:G:H5'	2.17	0.44
1:A:1372:U:OP1	9:I:71:SER:HB3	2.17	0.44
1:A:528:C:H5'	1:A:535:A:N6	2.32	0.44
1:A:596:C:O2'	1:A:597:G:H5'	2.16	0.44
2:B:27:LYS:HD2	2:B:193:ASP:OD1	2.17	0.44
2:B:77:ALA:CB	2:B:211:ILE:HD13	2.47	0.44
3:C:56:ASP:O	3:C:66:VAL:HA	2.17	0.44
6:F:68:PRO:HB2	6:F:71:ARG:CG	2.45	0.44
10:J:19:SER:OG	10:J:91:PRO:HG3	2.17	0.44
10:J:8:LEU:HD23	10:J:96:ILE:HG12	1.98	0.44
17:Q:68:ARG:O	17:Q:68:ARG:HG3	2.16	0.44
18:R:53:ARG:NH1	18:R:59:SER:HA	2.32	0.44
1:A:1183:A:O2'	1:A:1184:G:P	2.75	0.44
1:A:1289:A:H2'	1:A:1290:G:H5'	1.99	0.44
1:A:1337:G:H5"	1:A:1338:G:OP1	2.17	0.44
1:A:1426:C:O2'	1:A:1427:U:H5'	2.17	0.44
1:A:148:G:H2'	1:A:149:A:H8	1.83	0.44
1:A:1533:C:H5"	1:A:1533:C:C2	2.51	0.44
1:A:403:C:O3'	4:D:122:ARG:HD2	2.17	0.44
2:B:213:LEU:HD23	2:B:213:LEU:C	2.38	0.44
7:G:23:VAL:HG13	7:G:43:PHE:CE2	2.52	0.44
1:A:1231:G:C4'	9:I:126:SER:HB2	2.41	0.44
10:J:47:PHE:CE2	14:N:37:PHE:HE1	2.36	0.44
1:A:1524:C:OP1	11:K:120:ARG:NH1	2.49	0.44
1:A:552:U:H4'	12:L:86:ARG:O	2.17	0.44
17:Q:9:VAL:CG2	17:Q:84:LEU:HD13	2.48	0.44
1:A:1044:A:H2'	1:A:1045:C:H5'	1.99	0.44
1:A:1080:A:OP1	5:E:47:LYS:HE2	2.17	0.44
1:A:1229:A:C2	1:A:1230:C:C4	3.05	0.44
1:A:501:C:H2'	1:A:502:G:C8	2.52	0.44
1:A:730:G:C5	1:A:731:G:H1'	2.52	0.44
1:A:851:G:H2'	1:A:852:G:H8	1.83	0.44
1:A:954:G:H2'	1:A:955:U:C6	2.50	0.44
2:B:139:LYS:HE3	2:B:143:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:PHE:O	2:B:18:GLY:C	2.54	0.44
3:C:119:ARG:CG	3:C:140:ARG:HH12	2.28	0.44
3:C:66:VAL:O	3:C:66:VAL:HG12	2.16	0.44
4:D:4:TYR:O	4:D:5:ILE:HB	2.17	0.44
7:G:43:PHE:O	7:G:46:ALA:HB3	2.18	0.44
9:I:43:ALA:O	9:I:44:VAL:C	2.55	0.44
12:L:33:ARG:HG2	12:L:60:LEU:HG	1.98	0.44
13:M:23:TYR:C	13:M:25:ILE:H	2.21	0.44
13:M:81:LEU:HD23	13:M:81:LEU:N	2.31	0.44
19:S:33:THR:CG2	19:S:34:TRP:N	2.81	0.44
1:A:1007:C:H42	1:A:1022:G:H22	1.65	0.44
1:A:820:U:H4'	1:A:821:G:OP2	2.18	0.44
2:B:16:HIS:NE2	2:B:214:ILE:HD11	2.31	0.44
2:B:17:PHE:CD1	2:B:18:GLY:N	2.86	0.44
2:B:59:GLU:O	2:B:63:MET:HG2	2.18	0.44
5:E:72:GLN:O	5:E:73:ASN:CB	2.66	0.44
6:F:97:PHE:CE2	18:R:65:ILE:HD12	2.52	0.44
8:H:38:ILE:CG2	8:H:120:THR:HG22	2.48	0.44
2:B:181:PHE:CE2	8:H:70:GLN:HB3	2.52	0.44
9:I:99:LEU:N	9:I:99:LEU:HD22	2.32	0.44
11:K:108:ILE:HD12	18:R:88:LYS:HB3	2.00	0.44
16:P:59:TRP:HB3	16:P:64:ALA:HB2	1.99	0.44
17:Q:68:ARG:O	17:Q:69:LYS:HB2	2.18	0.44
17:Q:67:LYS:CA	17:Q:70:ARG:HH12	2.30	0.44
1:A:1005:A:H2'	1:A:1006:C:C5'	2.47	0.44
1:A:1054:C:H4'	1:A:1055:A:H5"	1.99	0.44
1:A:1343:G:H4'	9:I:122:ALA:O	2.17	0.44
1:A:138:G:O2'	1:A:139:G:H5'	2.18	0.44
1:A:157:G:H2'	1:A:158:G:H8	1.82	0.44
1:A:416:G:C6	1:A:417:C:C5	3.05	0.44
1:A:433:C:H5"	1:A:434:U:OP1	2.17	0.44
1:A:501:C:O2'	1:A:502:G:H5'	2.16	0.44
2:B:105:PHE:O	2:B:106:LYS:C	2.56	0.44
2:B:28:PHE:CZ	2:B:189:ASP:HA	2.53	0.44
3:C:145:GLY:O	3:C:146:ALA:HB3	2.17	0.44
3:C:154:SER:OG	3:C:196:LEU:HA	2.17	0.44
3:C:27:LYS:HA	3:C:30:ARG:HH12	1.82	0.44
4:D:36:ARG:HG2	4:D:38:TYR:OH	2.18	0.44
4:D:68:TYR:N	4:D:68:TYR:CD1	2.85	0.44
4:D:64:LEU:HD11	4:D:97:LEU:CD1	2.48	0.44
5:E:80:ILE:CD1	5:E:91:LEU:HD12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:26:ALA:CA	10:J:84:GLN:HE21	2.30	0.44
11:K:14:VAL:O	11:K:15:ALA:HB3	2.17	0.44
11:K:58:PRO:O	11:K:61:ALA:HB3	2.17	0.44
12:L:41:ARG:HG2	12:L:42:THR:O	2.18	0.44
14:N:22:THR:HB	14:N:33:VAL:HG21	1.98	0.44
17:Q:33:GLY:O	17:Q:34:LYS:C	2.56	0.44
18:R:19:LYS:HZ3	18:R:55:ARG:NH1	2.13	0.44
20:T:68:LYS:HA	20:T:68:LYS:HD2	1.80	0.44
1:A:1346:A:H1'	1:A:1347:G:OP2	2.18	0.44
1:A:1480:G:O2'	1:A:1481:U:H5'	2.18	0.44
1:A:1505:G:H3'	1:A:1505:G:C8	2.53	0.44
1:A:601:C:O2'	1:A:602:A:H5'	2.17	0.44
1:A:735:C:O2'	1:A:736:C:H5'	2.17	0.44
1:A:9:G:OP2	5:E:121:LYS:NZ	2.42	0.44
2:B:141:GLU:O	2:B:144:ARG:HG3	2.17	0.44
3:C:172:ARG:HB3	3:C:172:ARG:NH1	2.31	0.44
3:C:36:ASP:HB3	3:C:40:ARG:HH12	1.83	0.44
5:E:144:THR:HB	5:E:147:ASP:OD2	2.18	0.44
1:A:1128:C:C5'	9:I:16:ARG:NH1	2.81	0.44
9:I:49:PRO:O	9:I:52:ALA:HB3	2.17	0.44
9:I:4:TYR:CD2	9:I:88:TYR:HA	2.53	0.44
10:J:12:ASP:HB3	10:J:15:THR:CG2	2.48	0.44
10:J:47:PHE:HB2	10:J:63:PHE:HB2	1.99	0.44
12:L:115:LYS:O	12:L:117:ARG:N	2.44	0.44
12:L:86:ARG:HB3	12:L:101:VAL:CG2	2.47	0.44
13:M:20:THR:O	13:M:22:ILE:N	2.50	0.44
10:J:47:PHE:HD2	14:N:34:TYR:CD2	2.36	0.44
15:O:9:GLN:C	15:O:13:GLN:HE22	2.20	0.44
1:A:1326:C:H5"	21:U:12:LYS:HZ1	1.81	0.44
1:A:665:A:N3	1:A:732:C:H2'	2.33	0.44
1:A:737:A:H2'	1:A:738:C:C6	2.52	0.44
1:A:731:G:H5'	1:A:766:A:H4'	1.98	0.44
2:B:237:ALA:O	2:B:240:GLN:NE2	2.51	0.44
2:B:73:THR:HG22	2:B:169:LYS:NZ	2.33	0.44
3:C:204:LEU:O	3:C:205:GLY:O	2.35	0.44
10:J:44:VAL:HG21	10:J:66:ARG:HH21	1.82	0.44
11:K:48:ILE:CG1	11:K:64:ALA:HA	2.48	0.44
1:A:537:G:OP1	12:L:113:ARG:NH2	2.51	0.44
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.52	0.44
19:S:28:LYS:HD3	19:S:31:ILE:HD11	2.00	0.44
20:T:57:ARG:HH22	20:T:100:ILE:CD1	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:G:H4'	1:A:634:C:O2	2.17	0.44
1:A:1305:G:H22	1:A:1331:G:HO2'	1.64	0.44
1:A:1305:G:N2	1:A:1331:G:HO2'	2.14	0.44
1:A:552:U:O2	12:L:31:PRO:HB3	2.17	0.44
1:A:707:C:H2'	1:A:708:C:H6	1.83	0.44
1:A:858:G:O6	1:A:869:G:H3'	2.18	0.44
2:B:36:ARG:HD2	2:B:41:ILE:HD11	1.99	0.44
1:A:1060:C:C4	3:C:2:GLY:HA3	2.48	0.44
8:H:38:ILE:HG23	8:H:120:THR:HG22	2.00	0.44
13:M:82:MET:HE3	13:M:92:HIS:HB3	1.99	0.44
14:N:12:ARG:O	14:N:13:THR:C	2.55	0.44
19:S:29:ARG:H	19:S:29:ARG:CD	2.29	0.44
20:T:79:ARG:O	20:T:83:ARG:HG3	2.17	0.44
1:A:1305:G:N2	1:A:1331:G:C2'	2.81	0.44
1:A:162:A:C5	1:A:163:C:H1'	2.53	0.44
1:A:264:U:H4'	17:Q:63:ARG:HD3	2.00	0.44
1:A:46:G:O2'	1:A:365:U:H1'	2.18	0.44
1:A:560:U:H6	1:A:560:U:O5'	2.01	0.44
1:A:620:C:C2	4:D:135:LEU:HD13	2.52	0.44
1:A:951:G:O2'	1:A:952:U:H5'	2.18	0.44
5:E:151:LEU:CD2	8:H:79:VAL:HG22	2.47	0.44
10:J:38:ILE:HD12	10:J:71:LEU:HG	2.00	0.44
11:K:33:THR:HG22	11:K:39:PRO:CA	2.48	0.44
15:O:82:ILE:O	15:O:86:GLY:N	2.51	0.44
17:Q:78:GLU:O	17:Q:78:GLU:HG3	2.18	0.44
20:T:60:GLU:HG3	20:T:81:LYS:HE3	2.00	0.44
1:A:1353:G:H2'	1:A:1354:C:C6	2.53	0.43
1:A:482:A:H2'	1:A:483:C:O4'	2.17	0.43
2:B:144:ARG:HA	2:B:147:LYS:CD	2.48	0.43
3:C:157:ILE:HD13	3:C:166:GLU:HB2	1.99	0.43
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.51	0.43
9:I:80:GLY:O	9:I:83:ARG:N	2.51	0.43
9:I:85:LEU:HG	9:I:92:TYR:CD1	2.52	0.43
10:J:13:HIS:O	10:J:17:ASP:OD2	2.36	0.43
10:J:32:ALA:HB3	10:J:75:ILE:CG2	2.31	0.43
10:J:55:LYS:HG3	10:J:56:HIS:N	2.33	0.43
13:M:49:THR:CG2	13:M:51:ALA:HB3	2.48	0.43
13:M:94:ARG:HH11	13:M:94:ARG:HG3	1.82	0.43
19:S:74:PHE:N	19:S:74:PHE:CD1	2.86	0.43
1:A:1129:C:HO2'	1:A:1130:A:P	2.41	0.43
1:A:1055:A:C6	1:A:1206:G:C5	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:TRP:CG	3:C:59:ARG:HD2	2.53	0.43
4:D:199:ASN:HD21	4:D:201:GLN:HB2	1.82	0.43
4:D:24:GLU:OE1	4:D:25:ARG:N	2.37	0.43
7:G:15:ASP:OD2	7:G:23:VAL:HG11	2.18	0.43
8:H:103:VAL:HG21	8:H:109:ILE:C	2.37	0.43
9:I:99:LEU:CB	9:I:101:PHE:CE1	3.01	0.43
15:O:55:GLY:HA2	15:O:58:MET:CE	2.48	0.43
16:P:20:VAL:HG13	16:P:32:TYR:HB2	2.00	0.43
1:A:1085:U:H3'	1:A:1086:U:C5	2.53	0.43
1:A:129(A):G:C2	1:A:190(E):U:H5'	2.54	0.43
1:A:1347:G:H2'	1:A:1373:G:N1	2.33	0.43
1:A:247:G:C6	1:A:278:G:C2	3.07	0.43
1:A:538:G:OP2	12:L:115:LYS:HD2	2.17	0.43
3:C:36:ASP:O	3:C:39:ILE:HB	2.18	0.43
3:C:89:GLU:CG	3:C:93:LYS:HE2	2.49	0.43
8:H:31:PHE:HZ	8:H:134:ILE:HD11	1.82	0.43
10:J:75:ILE:HG12	10:J:76:ASN:ND2	2.33	0.43
12:L:111:LYS:O	12:L:112:ASP:HB2	2.18	0.43
12:L:55:VAL:CG1	12:L:56:ALA:H	2.20	0.43
14:N:14:PRO:CD	14:N:15:LYS:H	2.32	0.43
20:T:54:LYS:HA	20:T:57:ARG:HH12	1.83	0.43
21:U:6:ARG:HG3	21:U:7:ARG:N	2.33	0.43
1:A:1201:A:H4'	1:A:1202:G:O5'	2.18	0.43
1:A:1210:C:H5'	1:A:1214:C:N4	2.33	0.43
1:A:1279:A:H5"	1:A:1280:A:OP1	2.19	0.43
1:A:436:C:H2'	1:A:437:U:C6	2.53	0.43
1:A:457:C:O2'	1:A:458:C:H5'	2.17	0.43
1:A:55:A:C2	1:A:56:U:H1'	2.53	0.43
1:A:748:C:H1'	1:A:749:C:H5	1.83	0.43
2:B:17:PHE:HA	2:B:42:ILE:HB	2.01	0.43
2:B:74:LYS:HZ3	2:B:205:ASP:C	2.21	0.43
3:C:172:ARG:NH1	3:C:174:PRO:HG3	2.22	0.43
7:G:8:GLU:O	7:G:8:GLU:OE1	2.37	0.43
10:J:83:GLU:C	10:J:85:LEU:H	2.21	0.43
13:M:40:ASN:HD22	13:M:41:PRO:HD2	1.83	0.43
13:M:81:LEU:CD2	13:M:81:LEU:N	2.81	0.43
15:O:59:MET:HE2	15:O:59:MET:HB2	1.79	0.43
16:P:4:ILE:HA	16:P:20:VAL:O	2.17	0.43
17:Q:56:VAL:HG12	17:Q:77:VAL:HB	2.00	0.43
18:R:26:LEU:HD23	18:R:29:PHE:CE2	2.53	0.43
18:R:54:ARG:HH11	18:R:55:ARG:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:22:LEU:HD22	19:S:28:LYS:HD2	1.99	0.43
1:A:1003:G:C2	1:A:1003(A):G:C6	3.06	0.43
1:A:1251:A:H1'	1:A:1369:C:O2'	2.19	0.43
1:A:176:C:O2'	1:A:177:C:H5'	2.19	0.43
1:A:129(A):G:O2'	1:A:190(E):U:H2'	2.18	0.43
1:A:322:C:O2'	1:A:323:U:H5'	2.18	0.43
1:A:427:U:OP2	4:D:36:ARG:NH2	2.49	0.43
1:A:88:A:H2'	1:A:89:C:O4'	2.18	0.43
2:B:102:LEU:CD2	2:B:162:ILE:HD11	2.37	0.43
2:B:77:ALA:HB2	2:B:211:ILE:CD1	2.48	0.43
3:C:156:ARG:H	3:C:163:ALA:HA	1.84	0.43
4:D:32:ALA:C	4:D:34:GLU:H	2.21	0.43
4:D:32:ALA:C	4:D:34:GLU:N	2.71	0.43
5:E:99:GLY:O	5:E:117:ASP:HA	2.19	0.43
9:I:112:LYS:HD3	9:I:112:LYS:C	2.39	0.43
12:L:89:ARG:HG2	12:L:97:ARG:HA	2.00	0.43
17:Q:95:TYR:HD1	17:Q:95:TYR:N	2.17	0.43
1:A:1305:G:H22	1:A:1331:G:H2'	1.83	0.43
1:A:457:C:H2'	1:A:458:C:C6	2.53	0.43
1:A:685:G:H5'	11:K:39:PRO:O	2.18	0.43
1:A:980:C:H2'	1:A:981:U:O4'	2.19	0.43
2:B:24:TRP:HB3	2:B:40:HIS:CE1	2.54	0.43
3:C:21:ARG:HH22	3:C:56:ASP:CB	2.31	0.43
9:I:6:GLY:N	9:I:84:ALA:HB2	2.33	0.43
10:J:35:SER:OG	10:J:73:ASP:HB3	2.19	0.43
13:M:32:GLU:O	13:M:35:GLU:HB3	2.18	0.43
14:N:9:LYS:O	14:N:10:ALA:C	2.56	0.43
16:P:21:VAL:O	16:P:33:ILE:HB	2.18	0.43
16:P:39:TYR:CE2	16:P:41:PRO:HG3	2.54	0.43
17:Q:95:TYR:N	17:Q:95:TYR:CD1	2.85	0.43
19:S:62:ILE:HD12	19:S:63:THR:N	2.33	0.43
1:A:112:G:H21	1:A:354:G:C5'	2.24	0.43
1:A:1425:U:H3	1:A:1475:G:H1	1.65	0.43
1:A:918:A:H2'	1:A:919:A:C8	2.53	0.43
2:B:59:GLU:CB	2:B:221:LEU:HD11	2.46	0.43
3:C:34:LEU:C	3:C:34:LEU:CD2	2.81	0.43
4:D:199:ASN:C	4:D:199:ASN:HD22	2.21	0.43
5:E:12:LEU:C	5:E:12:LEU:HD22	2.39	0.43
5:E:40:ARG:NH1	5:E:40:ARG:HG2	2.34	0.43
5:E:82:VAL:HG11	5:E:137:GLU:HB3	2.01	0.43
8:H:63:LEU:HD22	8:H:63:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.21	0.43
9:I:89:ASN:O	9:I:92:TYR:HB2	2.18	0.43
13:M:67:GLU:O	13:M:70:LEU:N	2.50	0.43
1:A:1003(A):G:C4	1:A:1004:A:H1'	2.54	0.43
1:A:135:C:O2	16:P:1:MET:N	2.51	0.43
1:A:1511:G:O2'	1:A:1512:U:H5'	2.18	0.43
1:A:1527:C:H6	1:A:1527:C:O5'	2.02	0.43
1:A:384:G:H2'	1:A:385:C:H6	1.82	0.43
1:A:543:C:O2'	1:A:544:G:H5'	2.19	0.43
1:A:833:U:H2'	1:A:834:C:C6	2.54	0.43
4:D:111:ALA:HB2	4:D:120:LEU:HD12	2.01	0.43
4:D:15:GLU:CG	4:D:63:LYS:HG3	2.49	0.43
4:D:162:LEU:CD2	4:D:178:VAL:HG13	2.48	0.43
7:G:15:ASP:HB3	7:G:20:ASP:H	1.83	0.43
1:A:967:C:O2'	9:I:128:ARG:HD3	2.19	0.43
10:J:12:ASP:HB3	10:J:15:THR:CB	2.44	0.43
1:A:1038:C:H2'	1:A:1039:C:C5	2.51	0.43
1:A:1434:A:H2'	1:A:1435:G:O4'	2.19	0.43
1:A:203:U:C5'	1:A:204:U:OP1	2.66	0.43
1:A:586:C:O3'	8:H:89:PRO:HB2	2.18	0.43
1:A:984:C:H2'	1:A:985:C:C6	2.53	0.43
1:A:99:C:H2'	1:A:101:A:O4'	2.19	0.43
2:B:195:ASP:O	8:H:74:PRO:HG3	2.19	0.43
3:C:126:ARG:O	3:C:127:ARG:HB2	2.19	0.43
3:C:30:ARG:O	3:C:33:LEU:HB3	2.19	0.43
4:D:172:PRO:HG2	4:D:193:ASP:OD1	2.17	0.43
9:I:28:VAL:HA	9:I:63:ILE:O	2.19	0.43
9:I:8:GLY:HA2	9:I:79:LEU:HB3	2.00	0.43
11:K:93:GLN:NE2	11:K:96:ARG:HH21	2.15	0.43
12:L:38:THR:HB	12:L:39:VAL:H	1.64	0.43
12:L:85:ILE:CG2	12:L:98:TYR:HB3	2.48	0.43
1:A:1300:G:O2'	1:A:1301:U:H6	2.02	0.43
1:A:1404:C:H2'	1:A:1405:G:C8	2.54	0.43
1:A:171:A:O2'	1:A:172:A:H5'	2.19	0.43
1:A:397:A:H5'	1:A:398:C:P	2.59	0.43
1:A:39:G:O2'	1:A:40:C:H5'	2.19	0.43
1:A:554:C:H2'	1:A:555:C:C6	2.52	0.43
1:A:959:A:H2'	1:A:960:U:O4'	2.19	0.43
2:B:10:LEU:HG	2:B:48:MET:HE2	2.00	0.43
2:B:44:LEU:O	2:B:47:THR:HB	2.18	0.43
3:C:79:ARG:CG	3:C:82:GLU:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:64:ARG:H	5:E:64:ARG:HG2	1.44	0.43
6:F:8:ILE:HG23	6:F:85:VAL:HG13	2.00	0.43
7:G:15:ASP:HB3	7:G:19:GLY:N	2.34	0.43
9:I:40:LEU:C	9:I:42:ARG:N	2.73	0.43
10:J:12:ASP:OD1	10:J:14:LYS:N	2.52	0.43
10:J:38:ILE:HG13	10:J:71:LEU:HB3	2.01	0.43
11:K:34:ASP:HB2	11:K:35:PRO:HD2	2.01	0.43
14:N:14:PRO:O	14:N:15:LYS:HB3	2.18	0.43
16:P:40:ASP:HB3	16:P:48:TRP:HB2	2.01	0.43
19:S:18:LYS:O	19:S:22:LEU:HG	2.19	0.43
20:T:91:LEU:C	20:T:93:GLU:H	2.22	0.43
1:A:1005:A:H2'	1:A:1006:C:O4'	2.18	0.42
1:A:1096:C:H2'	1:A:1097:C:C6	2.50	0.42
2:B:193:ASP:HA	2:B:194:PRO:HD2	1.85	0.42
3:C:139:GLN:O	3:C:143:GLU:HB2	2.19	0.42
6:F:91:VAL:HG11	18:R:72:ARG:HH12	1.83	0.42
8:H:102:ARG:HG2	8:H:125:ARG:HH12	1.84	0.42
11:K:108:ILE:O	11:K:109:VAL:HG23	2.19	0.42
11:K:12:ARG:H	11:K:13:GLN:NE2	2.17	0.42
17:Q:67:LYS:O	17:Q:68:ARG:C	2.55	0.42
6:F:62:TRP:CG	18:R:35:ARG:NH1	2.87	0.42
20:T:50:GLU:O	20:T:100:ILE:HG21	2.19	0.42
1:A:1235:U:H2'	1:A:1236:A:O4'	2.19	0.42
1:A:131:C:H2'	1:A:132:C:H6	1.84	0.42
1:A:485:G:O2'	1:A:486:U:OP2	2.37	0.42
1:A:542:G:H2'	1:A:543:C:H6	1.84	0.42
1:A:725:G:O2'	1:A:726:C:H5'	2.18	0.42
1:A:855:G:H2'	1:A:856:C:C6	2.54	0.42
2:B:16:HIS:HA	2:B:204:ASN:CG	2.38	0.42
3:C:139:GLN:NE2	3:C:139:GLN:HA	2.34	0.42
3:C:67:THR:O	3:C:69:HIS:CD2	2.72	0.42
4:D:2:GLY:O	4:D:4:TYR:N	2.52	0.42
7:G:72:ARG:HA	7:G:96:GLN:HE21	1.81	0.42
9:I:78:LYS:HD3	9:I:101:PHE:HD2	1.83	0.42
15:O:17:ARG:O	15:O:18:PHE:HB3	2.19	0.42
16:P:8:ARG:HB2	16:P:28:ARG:NH1	2.33	0.42
17:Q:40:LYS:HG2	17:Q:41:LYS:N	2.34	0.42
1:A:1392:G:H2'	1:A:1393:U:C6	2.54	0.42
1:A:1402:C:O2	1:A:1500:A:N1	2.52	0.42
1:A:1474:G:H2'	1:A:1475:G:H8	1.84	0.42
1:A:19:C:O2'	1:A:20:U:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:C:H2'	1:A:690:G:O4'	2.19	0.42
2:B:189:ASP:HB3	2:B:203:GLY:O	2.18	0.42
2:B:36:ARG:CD	2:B:41:ILE:HD12	2.49	0.42
2:B:60:ASP:OD1	2:B:64:ARG:NH2	2.52	0.42
2:B:98:LEU:CD2	2:B:98:LEU:H	2.32	0.42
10:J:34:VAL:CG2	10:J:74:ILE:HG23	2.38	0.42
12:L:119:LYS:C	12:L:121:GLY:H	2.23	0.42
18:R:19:LYS:HE2	18:R:55:ARG:HD2	2.00	0.42
1:A:1168:A:C6	1:A:1169:A:C6	3.07	0.42
1:A:1189:C:OP2	10:J:51:ARG:NH2	2.53	0.42
1:A:142:G:N3	1:A:196:A:C2	2.88	0.42
1:A:707:C:H5"	11:K:20:TYR:CD2	2.54	0.42
1:A:840:C:H4'	1:A:841:U:O5'	2.18	0.42
3:C:58:GLU:O	3:C:64:VAL:HA	2.18	0.42
5:E:13:ILE:O	5:E:13:ILE:HG13	2.18	0.42
8:H:39:LEU:HA	8:H:39:LEU:HD13	1.76	0.42
14:N:23:ARG:HA	14:N:29:ARG:O	2.19	0.42
15:O:74:ASP:CG	15:O:77:ARG:HG3	2.40	0.42
1:A:112:G:O2'	1:A:113:G:H5'	2.20	0.42
1:A:1305:G:O2'	1:A:1306:A:C8	2.47	0.42
1:A:1347:G:C2'	1:A:1373:G:H1	2.31	0.42
1:A:1513:A:H2'	1:A:1514:C:C6	2.54	0.42
1:A:1533:C:O2	1:A:1533:C:C2'	2.67	0.42
1:A:166:G:H2'	1:A:167:G:H8	1.84	0.42
1:A:364:A:N6	12:L:28:LYS:HE2	2.34	0.42
4:D:142:PRO:HA	4:D:185:PHE:O	2.19	0.42
5:E:96:PRO:HA	5:E:117:ASP:OD2	2.20	0.42
8:H:9:MET:SD	8:H:32:LYS:HB3	2.60	0.42
9:I:28:VAL:HG22	9:I:63:ILE:HB	2.00	0.42
9:I:33:PHE:CE2	9:I:47:LEU:HD11	2.55	0.42
10:J:10:GLY:N	10:J:16:LEU:HD21	2.35	0.42
10:J:34:VAL:N	10:J:75:ILE:HG22	2.34	0.42
10:J:47:PHE:N	10:J:63:PHE:O	2.49	0.42
10:J:71:LEU:O	10:J:72:VAL:HB	2.18	0.42
12:L:42:THR:CG2	12:L:52:LEU:HB3	2.48	0.42
12:L:54:LYS:N	12:L:54:LYS:CD	2.83	0.42
17:Q:82:MET:O	17:Q:86:GLU:HB2	2.19	0.42
19:S:28:LYS:HD3	19:S:31:ILE:CD1	2.49	0.42
1:A:1417:G:H2'	1:A:1482:G:N2	2.34	0.42
1:A:304:U:H2'	1:A:305:G:C8	2.55	0.42
3:C:52:LEU:N	3:C:52:LEU:CD2	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:6:GLY:H	4:D:115:ARG:HH22	1.68	0.42
8:H:29:SER:O	8:H:30:ARG:C	2.58	0.42
9:I:118:LYS:O	9:I:120:ARG:N	2.46	0.42
1:A:1128:C:H5'	9:I:16:ARG:NH1	2.35	0.42
14:N:5:ALA:O	14:N:8:GLU:CG	2.67	0.42
20:T:69:GLY:O	20:T:73:HIS:CD2	2.73	0.42
1:A:1085:U:H3'	1:A:1086:U:H5	1.85	0.42
1:A:1154:G:H2'	1:A:1155:G:H8	1.84	0.42
1:A:1014:A:H2	1:A:1219:U:H1'	1.83	0.42
1:A:194:C:OP1	20:T:61:SER:OG	2.30	0.42
1:A:258:G:H2'	1:A:259:G:H8	1.85	0.42
1:A:322:C:H41	1:A:328:C:H6	1.68	0.42
1:A:854:G:C6	1:A:855:G:N7	2.87	0.42
2:B:153:ARG:HG2	2:B:153:ARG:HH11	1.85	0.42
2:B:33:TYR:HB2	2:B:43:ASP:HA	2.01	0.42
3:C:119:ARG:O	3:C:122:GLU:HB2	2.20	0.42
3:C:134:ILE:O	3:C:138:VAL:HG23	2.20	0.42
3:C:22:TRP:O	3:C:22:TRP:CE3	2.73	0.42
3:C:23:TYR:CZ	3:C:24:ALA:O	2.72	0.42
4:D:70:ILE:HG22	4:D:74:GLN:HB2	2.00	0.42
4:D:68:TYR:CE2	4:D:97:LEU:HB3	2.54	0.42
8:H:82:HIS:O	8:H:83:ILE:CB	2.67	0.42
1:A:1128:C:C4'	9:I:16:ARG:HH12	2.32	0.42
10:J:32:ALA:O	10:J:34:VAL:HG23	2.19	0.42
12:L:110:VAL:O	12:L:122:THR:CG2	2.67	0.42
12:L:24:VAL:N	12:L:25:PRO:HD3	2.33	0.42
13:M:35:GLU:C	13:M:37:THR:H	2.23	0.42
13:M:2:ALA:O	13:M:4:ILE:HG13	2.20	0.42
14:N:45:ARG:O	14:N:49:HIS:CD2	2.72	0.42
17:Q:34:LYS:HG3	17:Q:34:LYS:O	2.19	0.42
1:A:1394:A:C6	1:A:1501:C:H4'	2.55	0.42
1:A:794:A:H2'	1:A:795:C:O4'	2.19	0.42
1:A:895:G:H2'	1:A:896:C:H6	1.81	0.42
2:B:134:GLU:C	2:B:136:VAL:N	2.73	0.42
2:B:71:VAL:O	2:B:165:VAL:HG23	2.20	0.42
2:B:167:PRO:HG3	2:B:188:ALA:CB	2.48	0.42
2:B:92:TYR:CD1	2:B:92:TYR:C	2.93	0.42
3:C:155:GLY:O	3:C:156:ARG:CB	2.68	0.42
3:C:22:TRP:CH2	3:C:32:LEU:HB2	2.55	0.42
5:E:145:LYS:O	5:E:149:GLU:HB2	2.19	0.42
5:E:18:ARG:HE	5:E:18:ARG:HB3	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:50:ILE:HG12	7:G:125:MET:CE	2.50	0.42
9:I:10:ARG:HG2	9:I:75:ASP:HB2	2.00	0.42
1:A:1125:U:H3	10:J:5:ARG:HE	1.66	0.42
12:L:41:ARG:CG	12:L:42:THR:N	2.70	0.42
13:M:125:ARG:HH11	13:M:126:LYS:HA	1.85	0.42
13:M:67:GLU:O	13:M:68:GLY:C	2.58	0.42
18:R:71:LYS:O	18:R:75:ILE:HG13	2.20	0.42
1:A:119:A:H4'	1:A:120:A:O5'	2.18	0.42
1:A:544:G:OP2	4:D:66:ARG:NH2	2.53	0.42
1:A:824:C:H2'	1:A:825:G:C8	2.55	0.42
2:B:209:ARG:HG2	2:B:209:ARG:HH11	1.85	0.42
2:B:25:ASN:ND2	2:B:25:ASN:C	2.71	0.42
2:B:95:GLN:O	2:B:96:ARG:NE	2.53	0.42
3:C:134:ILE:HG21	3:C:167:TRP:O	2.20	0.42
5:E:152:ARG:C	8:H:64:LYS:NZ	2.73	0.42
6:F:24:GLU:O	6:F:28:ARG:HB2	2.19	0.42
9:I:8:GLY:CA	9:I:79:LEU:HB3	2.50	0.42
13:M:82:MET:HA	13:M:89:GLY:HA3	2.01	0.42
1:A:1129:C:O2'	1:A:1130:A:OP2	2.34	0.42
1:A:22:G:H2'	1:A:23:C:C6	2.55	0.42
1:A:442:C:H2'	1:A:444:C:H42	1.84	0.42
1:A:938:A:C6	1:A:939:G:C5	3.08	0.42
2:B:108:ILE:O	2:B:108:ILE:CG2	2.68	0.42
3:C:132:ARG:O	3:C:136:GLN:HG3	2.20	0.42
5:E:74:GLY:CA	5:E:116:THR:HG22	2.50	0.42
6:F:3:ARG:NH2	6:F:38:GLU:OE2	2.53	0.42
6:F:53:ALA:C	6:F:54:LYS:HG2	2.40	0.42
7:G:52:GLU:O	7:G:54:THR:N	2.53	0.42
8:H:45:ILE:O	8:H:46:LYS:C	2.58	0.42
9:I:55:ALA:O	9:I:56:LEU:CB	2.67	0.42
12:L:126:LYS:CA	12:L:126:LYS:HE3	2.50	0.42
12:L:41:ARG:HH12	12:L:57:LYS:HZ1	1.68	0.42
14:N:25:VAL:O	14:N:25:VAL:HG22	2.19	0.42
14:N:3:ARG:O	14:N:4:LYS:C	2.58	0.42
16:P:4:ILE:O	16:P:66:PRO:HA	2.20	0.42
19:S:77:THR:HG22	19:S:78:ARG:N	2.34	0.42
1:A:1004:A:N7	1:A:1036:G:O6	2.53	0.41
1:A:115:G:H1'	1:A:116:A:N7	2.35	0.41
1:A:959:A:C2	1:A:1222:G:O4'	2.73	0.41
1:A:1236:A:OP1	21:U:2:GLY:HA3	2.20	0.41
1:A:1346:A:C5	7:G:10:ARG:NH2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:C:O2'	1:A:380:G:H5'	2.19	0.41
1:A:402:G:O2'	1:A:403:C:H5'	2.20	0.41
1:A:625:G:H2'	1:A:626:U:C6	2.55	0.41
3:C:5:ILE:HD13	3:C:10:PHE:HB2	2.02	0.41
4:D:31:CYS:O	4:D:33:MET:N	2.50	0.41
5:E:15:ARG:HD2	5:E:15:ARG:C	2.40	0.41
8:H:83:ILE:CG2	8:H:83:ILE:O	2.64	0.41
1:A:1249:C:H4'	9:I:36:TYR:OH	2.20	0.41
9:I:3:GLN:HG3	9:I:20:ARG:CG	2.50	0.41
9:I:75:ASP:O	9:I:78:LYS:HB3	2.19	0.41
10:J:82:ILE:O	10:J:82:ILE:HG22	2.20	0.41
15:O:66:LEU:O	15:O:69:TYR:HB3	2.20	0.41
18:R:68:LYS:O	18:R:72:ARG:HG3	2.20	0.41
21:U:2:GLY:C	21:U:4:GLY:N	2.73	0.41
1:A:1256:A:H5'	1:A:1258:G:C1'	2.47	0.41
1:A:1307:U:H2'	1:A:1308:U:H6	1.83	0.41
1:A:1401:G:H2'	1:A:1402:C:O4'	2.20	0.41
1:A:1499:A:C2	1:A:1500:A:C8	3.07	0.41
1:A:28:G:O2'	1:A:296:U:OP1	2.38	0.41
1:A:327:A:H3'	1:A:328:C:H5"	2.02	0.41
2:B:16:HIS:N	2:B:204:ASN:HD21	2.16	0.41
2:B:21:ARG:HB2	2:B:22:LYS:H	1.55	0.41
3:C:95:THR:HB	3:C:97:LYS:HG2	2.01	0.41
5:E:82:VAL:HG21	5:E:138:ALA:HA	2.01	0.41
17:Q:101:ARG:HE	17:Q:101:ARG:HA	1.85	0.41
17:Q:68:ARG:NH1	17:Q:68:ARG:HG2	2.27	0.41
20:T:11:SER:O	20:T:13:LEU:HD12	2.19	0.41
20:T:39:LYS:CD	20:T:55:ILE:HD13	2.51	0.41
1:A:1179:A:H2'	1:A:1180:A:O4'	2.21	0.41
1:A:1251:A:H5'	9:I:12:GLU:OE1	2.20	0.41
1:A:1273:G:H2'	1:A:1274:G:O4'	2.20	0.41
1:A:1425:U:H2'	1:A:1426:C:H6	1.79	0.41
1:A:146:G:O2'	1:A:147:G:H5'	2.20	0.41
1:A:419:C:OP1	1:A:513:C:H1'	2.20	0.41
1:A:50:A:H4'	1:A:51:A:H5'	2.02	0.41
1:A:605:U:O2'	1:A:606:G:H5'	2.21	0.41
1:A:953:G:H2'	1:A:954:G:O4'	2.20	0.41
1:A:1060:C:H5	3:C:2:GLY:HA3	1.71	0.41
3:C:75:VAL:O	3:C:83:ARG:NH1	2.54	0.41
4:D:126:ILE:HG22	4:D:127:THR:N	2.36	0.41
7:G:156:TRP:HE3	7:G:156:TRP:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:152:ARG:NH2	8:H:107:LEU:O	2.52	0.41
8:H:88:LYS:HB3	8:H:89:PRO:HD2	2.01	0.41
9:I:43:ALA:O	9:I:45:ALA:N	2.53	0.41
12:L:39:VAL:HG12	12:L:40:VAL:N	2.35	0.41
12:L:83:VAL:HG11	12:L:100:ILE:CD1	2.49	0.41
1:A:267:C:P	17:Q:67:LYS:HB2	2.60	0.41
1:A:1314:C:N4	19:S:4:SER:OG	2.52	0.41
1:A:1060:C:O2'	1:A:1061:G:H5'	2.21	0.41
1:A:1110:A:O5'	1:A:1110:A:H8	2.02	0.41
1:A:270:A:H2'	1:A:271:C:C6	2.56	0.41
3:C:191:THR:HG22	3:C:192:THR:N	2.32	0.41
5:E:149:GLU:HG2	5:E:153:LYS:HE2	2.02	0.41
2:B:178:ARG:NH1	8:H:71:GLY:O	2.54	0.41
10:J:16:LEU:HD23	10:J:94:VAL:CG2	2.49	0.41
10:J:4:ILE:HG13	10:J:74:ILE:O	2.20	0.41
17:Q:12:SER:HB3	17:Q:20:THR:CB	2.50	0.41
21:U:24:ARG:N	21:U:24:ARG:CD	2.84	0.41
1:A:192:U:O3'	20:T:57:ARG:HD2	2.21	0.41
1:A:416:G:O2'	1:A:417:C:H5'	2.21	0.41
1:A:562:C:H1'	12:L:15:ARG:HB3	2.01	0.41
2:B:118:LEU:CB	2:B:142:LEU:HD21	2.51	0.41
2:B:54:THR:O	2:B:58:ILE:HG13	2.20	0.41
3:C:179:ARG:HD3	3:C:206:GLU:HG2	2.03	0.41
3:C:47:LEU:CD2	3:C:68:VAL:HG11	2.50	0.41
3:C:50:ALA:O	3:C:70:VAL:CG1	2.69	0.41
4:D:187:ARG:HD2	4:D:188:LEU:N	2.30	0.41
4:D:187:ARG:CG	4:D:188:LEU:N	2.83	0.41
5:E:81:GLU:CD	5:E:88:LYS:HE2	2.40	0.41
9:I:9:ARG:CG	9:I:14:VAL:HG22	2.51	0.41
10:J:34:VAL:HA	10:J:75:ILE:H	1.85	0.41
10:J:23:ILE:HG21	10:J:72:VAL:HG11	2.03	0.41
1:A:981:U:H5'	14:N:21:TYR:CE1	2.55	0.41
15:O:64:ARG:HG2	15:O:64:ARG:H	1.73	0.41
15:O:71:GLN:HB2	15:O:78:TYR:CD1	2.55	0.41
19:S:12:ASP:H	19:S:38:SER:CB	2.31	0.41
1:A:1262:C:O2'	1:A:1263:C:H5'	2.21	0.41
1:A:1392:G:H2'	1:A:1393:U:H6	1.86	0.41
1:A:299:G:H2'	1:A:300:A:C8	2.56	0.41
2:B:116:GLU:HG2	2:B:153:ARG:NH1	2.33	0.41
3:C:191:THR:HB	3:C:194:GLY:O	2.20	0.41
4:D:159:ARG:HD3	4:D:159:ARG:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:ARG:O	4:D:36:ARG:CG	2.69	0.41
5:E:100:VAL:O	5:E:107:ARG:NH2	2.46	0.41
6:F:101:ALA:HA	18:R:28:GLU:CG	2.45	0.41
7:G:54:THR:CG2	7:G:55:GLY:H	2.20	0.41
10:J:5:ARG:HB2	10:J:99:LYS:O	2.20	0.41
10:J:26:ALA:O	10:J:85:LEU:HG	2.20	0.41
11:K:77:MET:HB3	11:K:103:LEU:HD21	2.02	0.41
18:R:36:ASN:C	18:R:36:ASN:ND2	2.73	0.41
18:R:39:VAL:HG13	18:R:40:LEU:N	2.34	0.41
20:T:87:LYS:HE3	20:T:87:LYS:HB2	1.79	0.41
1:A:101:A:H2'	1:A:102:G:H8	1.86	0.41
1:A:722:A:O2'	1:A:723:U:C2	2.74	0.41
1:A:722:A:H5'	1:A:723:U:OP1	2.21	0.41
2:B:16:HIS:HB3	2:B:17:PHE:H	1.63	0.41
2:B:30:ARG:HD2	2:B:31:TYR:CE2	2.56	0.41
2:B:75:LYS:O	2:B:76:GLN:C	2.58	0.41
2:B:87:ARG:NH2	2:B:233:SER:HB2	2.36	0.41
4:D:153:ARG:HG3	4:D:181:MET:SD	2.61	0.41
6:F:100:ASN:HA	18:R:23:LYS:CE	2.44	0.41
6:F:28:ARG:HG3	6:F:28:ARG:HH11	1.86	0.41
6:F:4:TYR:CE2	6:F:72:VAL:CG2	3.03	0.41
8:H:34:GLU:O	8:H:38:ILE:HD12	2.21	0.41
10:J:34:VAL:H	10:J:75:ILE:CG2	2.33	0.41
12:L:126:LYS:O	12:L:127:GLU:C	2.58	0.41
13:M:20:THR:C	13:M:22:ILE:N	2.74	0.41
15:O:70:LEU:HD11	15:O:77:ARG:CB	2.51	0.41
16:P:1:MET:HE2	16:P:3:LYS:CG	2.51	0.41
18:R:34:TYR:HA	18:R:69:THR:HG23	2.01	0.41
18:R:48:GLY:O	18:R:74:ARG:NH2	2.54	0.41
1:A:1056:U:H5'	3:C:163:ALA:CB	2.50	0.41
1:A:1197:G:O2'	1:A:1198:G:H5'	2.20	0.41
1:A:1320:C:O2'	1:A:1321:C:H5'	2.21	0.41
1:A:1341:U:O2'	1:A:1342:C:H5'	2.21	0.41
1:A:1360:A:O2'	1:A:1361:G:H5'	2.21	0.41
1:A:254:G:O2'	1:A:255:G:H5'	2.20	0.41
1:A:414:A:H2'	1:A:416:G:H1	1.85	0.41
1:A:584:G:H2'	1:A:585:G:C8	2.56	0.41
1:A:836:G:H2'	1:A:837:G:H8	1.86	0.41
1:A:575:G:C5	1:A:881:G:C2	3.09	0.41
2:B:114:ARG:HH11	2:B:118:LEU:CG	2.34	0.41
2:B:121:LEU:HD22	2:B:126:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:ARG:O	2:B:158:LEU:C	2.59	0.41
2:B:7:VAL:O	2:B:7:VAL:HG23	2.20	0.41
4:D:189:PRO:HB2	4:D:194:LEU:CD2	2.51	0.41
1:A:1194:U:H4'	5:E:22:GLY:HA2	2.02	0.41
7:G:85:TYR:O	7:G:87:VAL:HG23	2.20	0.41
11:K:116:HIS:O	11:K:117:ASN:HB2	2.21	0.41
12:L:38:THR:HB	12:L:57:LYS:HB2	2.02	0.41
13:M:98:VAL:O	13:M:98:VAL:HG12	2.21	0.41
15:O:39:LEU:HD11	15:O:56:LEU:HB2	1.98	0.41
15:O:70:LEU:HD12	15:O:78:TYR:HA	2.01	0.41
15:O:74:ASP:OD1	15:O:76:GLU:HB3	2.21	0.41
20:T:72:LEU:O	20:T:73:HIS:C	2.59	0.41
1:A:1125:U:H5"	1:A:1126:U:C5	2.56	0.41
1:A:1396:A:H4'	1:A:1397:C:H5"	2.03	0.41
1:A:462:G:O2'	1:A:463:A:H5'	2.21	0.41
3:C:116:VAL:O	3:C:120:VAL:HG23	2.21	0.41
11:K:84:VAL:CG2	11:K:110:ASP:HA	2.45	0.41
15:O:45:VAL:HB	15:O:46:HIS:ND1	2.35	0.41
16:P:82:GLN:O	16:P:83:GLU:C	2.58	0.41
17:Q:68:ARG:N	17:Q:70:ARG:HH12	2.19	0.41
1:A:1136:U:H5"	1:A:1137:C:OP2	2.20	0.41
1:A:1145:C:O2'	1:A:1146:A:O5'	2.35	0.41
1:A:244:U:O4	1:A:906:G:H1'	2.21	0.41
1:A:957:U:H3	1:A:960:U:C5'	2.34	0.41
2:B:230:VAL:CG1	2:B:231:GLU:N	2.84	0.41
2:B:24:TRP:CZ3	2:B:29:ALA:HB2	2.55	0.41
3:C:107:GLN:NE2	3:C:107:GLN:H	2.18	0.41
3:C:139:GLN:HE21	3:C:139:GLN:CA	2.34	0.41
3:C:39:ILE:HG22	3:C:40:ARG:N	2.36	0.41
3:C:47:LEU:H	3:C:47:LEU:CD1	2.34	0.41
4:D:76:ARG:HH11	4:D:76:ARG:HG2	1.86	0.41
8:H:17:THR:HB	8:H:78:GLN:OE1	2.21	0.41
14:N:9:LYS:C	14:N:11:LYS:N	2.73	0.41
16:P:40:ASP:HB3	16:P:48:TRP:CB	2.51	0.41
17:Q:5:VAL:HG22	17:Q:60:ILE:HG12	2.02	0.41
1:A:1260:C:H4'	1:A:1283:G:O2'	2.20	0.41
1:A:1413:A:H2'	1:A:1414:U:O4'	2.21	0.41
1:A:1416:G:H2'	1:A:1417:G:H5'	2.03	0.41
1:A:162:A:H2'	1:A:163:C:O4'	2.20	0.41
1:A:298:A:H2'	1:A:299:G:O4'	2.21	0.41
1:A:429:U:H4'	1:A:430:A:O5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:U:H2'	1:A:637:G:C8	2.55	0.41
2:B:77:ALA:CB	2:B:211:ILE:CD1	2.99	0.41
2:B:68:ILE:HB	2:B:90:MET:CE	2.51	0.41
1:A:409:G:OP1	4:D:25:ARG:HB2	2.21	0.41
4:D:25:ARG:HG2	4:D:25:ARG:HH11	1.85	0.41
5:E:62:ALA:O	5:E:64:ARG:O	2.39	0.41
7:G:75:VAL:HG22	7:G:86:GLN:HB3	2.03	0.41
8:H:87:SER:HA	8:H:93:VAL:HG23	2.03	0.41
9:I:31:GLN:HB3	9:I:35:GLU:HB3	2.03	0.41
12:L:93:LEU:HD23	12:L:93:LEU:N	2.35	0.41
14:N:23:ARG:HG2	14:N:23:ARG:NH1	2.36	0.41
19:S:13:ASP:O	19:S:14:HIS:C	2.58	0.41
19:S:20:LEU:HA	19:S:23:ASN:HD22	1.83	0.41
19:S:32:LYS:HA	19:S:50:ALA:HB3	2.03	0.41
1:A:1021:G:O2'	1:A:1022:G:H5'	2.21	0.40
1:A:1090:U:H2'	1:A:1091:U:C6	2.55	0.40
1:A:1095:U:H2'	1:A:1096:C:O4'	2.20	0.40
1:A:1095:U:H5"	1:A:1109:C:O2	2.20	0.40
1:A:1183:A:O2'	1:A:1184:G:OP1	2.38	0.40
1:A:1194:U:H2'	1:A:1195:C:C6	2.56	0.40
1:A:1278:U:H5	10:J:97:GLU:OE1	2.05	0.40
1:A:1239:A:H62	1:A:1299:A:H62	1.69	0.40
1:A:130:A:H1'	1:A:263:A:O2'	2.21	0.40
1:A:342:C:H2'	1:A:343:U:H5'	2.03	0.40
1:A:67:C:H2'	1:A:68:G:C8	2.57	0.40
1:A:909:A:H2'	1:A:910:C:O4'	2.20	0.40
1:A:942:G:H2'	1:A:943:U:C6	2.54	0.40
2:B:54:THR:O	2:B:57:PHE:HB3	2.21	0.40
3:C:21:ARG:HG3	3:C:58:GLU:HG2	2.03	0.40
3:C:72:LYS:HB3	3:C:75:VAL:HG23	2.04	0.40
9:I:10:ARG:O	9:I:11:LYS:C	2.59	0.40
11:K:81:ASP:OD2	11:K:106:LYS:HB2	2.21	0.40
13:M:11:ARG:O	13:M:12:ASN:C	2.60	0.40
18:R:43:PHE:C	18:R:51:LEU:HD12	2.42	0.40
19:S:63:THR:H	19:S:66:MET:CG	2.33	0.40
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.56	0.40
1:A:414:A:H5'	1:A:415:A:OP1	2.21	0.40
1:A:578:C:H2'	1:A:579:G:O4'	2.21	0.40
1:A:694:A:C2'	1:A:695:A:O5'	2.69	0.40
2:B:106:LYS:O	2:B:109:SER:OG	2.35	0.40
2:B:122:PHE:CE2	2:B:139:LYS:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:GLY:N	2:B:41:ILE:HA	2.36	0.40
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.56	0.40
4:D:56:VAL:HG12	4:D:202:LEU:HD13	2.04	0.40
4:D:62:GLN:CA	4:D:62:GLN:HE21	2.28	0.40
5:E:69:VAL:HG21	5:E:113:ALA:HB1	2.04	0.40
5:E:93:PRO:HG2	8:H:105:ARG:CZ	2.51	0.40
9:I:24:GLY:O	9:I:26:VAL:HG23	2.21	0.40
10:J:83:GLU:C	10:J:85:LEU:N	2.74	0.40
11:K:15:ALA:HA	11:K:76:GLY:O	2.21	0.40
12:L:37:CYS:O	12:L:79:GLU:O	2.39	0.40
13:M:107:ALA:O	13:M:111:LYS:HG3	2.22	0.40
14:N:27:CYS:SG	14:N:29:ARG:N	2.89	0.40
14:N:34:TYR:N	14:N:34:TYR:CD1	2.89	0.40
1:A:191:G:N3	20:T:105:SER:HB3	2.37	0.40
20:T:93:GLU:HA	20:T:93:GLU:OE1	2.21	0.40
1:A:1347:G:OP2	1:A:1347:G:O4'	2.39	0.40
1:A:1367:C:C2	1:A:1368:G:C8	3.09	0.40
1:A:1486:G:H2'	1:A:1487:G:C8	2.57	0.40
1:A:1495:U:H2'	1:A:1496:C:H6	1.86	0.40
6:F:27:GLN:O	6:F:31:GLU:HG3	2.21	0.40
7:G:104:LEU:HA	7:G:104:LEU:HD23	1.90	0.40
9:I:4:TYR:O	9:I:18:PHE:HA	2.21	0.40
9:I:48:GLU:OE1	9:I:48:GLU:HA	2.21	0.40
9:I:43:ALA:HA	9:I:74:ILE:HD13	2.03	0.40
13:M:90:LEU:O	13:M:93:ARG:HB2	2.22	0.40
18:R:19:LYS:O	18:R:20:ALA:CB	2.69	0.40
18:R:19:LYS:HE2	18:R:55:ARG:CD	2.52	0.40
20:T:45:GLN:C	20:T:47:GLY:N	2.74	0.40
20:T:73:HIS:HB3	20:T:74:LYS:H	1.62	0.40
1:A:1057:G:O2'	1:A:1058:G:H5'	2.21	0.40
1:A:1072:G:H2'	1:A:1073:U:H6	1.79	0.40
1:A:216:G:H2'	1:A:217:C:C6	2.57	0.40
1:A:397:A:H5'	1:A:398:C:OP1	2.22	0.40
1:A:56:U:H2'	1:A:57:G:H8	1.85	0.40
1:A:633:G:H2'	1:A:634:C:C6	2.56	0.40
2:B:88:ALA:HB1	2:B:90:MET:HG2	2.04	0.40
3:C:59:ARG:NH1	3:C:64:VAL:HG22	2.37	0.40
3:C:91:LEU:C	3:C:91:LEU:HD23	2.41	0.40
4:D:100:ARG:NH1	4:D:137:SER:HB3	2.36	0.40
5:E:80:ILE:O	5:E:80:ILE:HD12	2.21	0.40
11:K:82:VAL:HG23	11:K:105:VAL:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:40:ASN:ND2	13:M:40:ASN:C	2.74	0.40
13:M:97:PRO:HB2	13:M:101:GLN:OE1	2.22	0.40
14:N:9:LYS:HE3	14:N:21:TYR:O	2.21	0.40
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	2.02	0.40
20:T:62:LEU:HA	20:T:62:LEU:HD23	1.88	0.40
1:A:1067:A:O2'	1:A:1093:A:O3'	2.37	0.40
1:A:114:U:H2'	1:A:115:G:C8	2.57	0.40
1:A:1227:A:C4	19:S:81:ARG:NH1	2.85	0.40
1:A:315:A:O4'	1:A:353:A:C2	2.74	0.40
1:A:386:C:O2'	1:A:387:U:H5'	2.21	0.40
1:A:112:G:C5'	1:A:389:A:H4'	2.51	0.40
1:A:5:U:H4'	1:A:6:G:C5'	2.51	0.40
1:A:746:A:C2'	1:A:747:C:H5'	2.52	0.40
2:B:73:THR:HG23	2:B:95:GLN:O	2.21	0.40
3:C:39:ILE:C	3:C:41:GLY:N	2.74	0.40
3:C:36:ASP:HB3	3:C:40:ARG:NH1	2.36	0.40
4:D:191:ARG:HD2	4:D:191:ARG:HA	1.92	0.40
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.99	0.40
5:E:11:ILE:HD11	5:E:33:VAL:HG21	2.03	0.40
7:G:17:VAL:CG1	7:G:18:TYR:CD1	3.05	0.40
9:I:48:GLU:OE1	9:I:51:ARG:HB2	2.22	0.40
9:I:69:GLY:O	9:I:73:GLN:HG3	2.21	0.40
10:J:69:ASN:C	10:J:70:ARG:HE	2.25	0.40
12:L:41:ARG:CB	12:L:41:ARG:NH1	2.85	0.40
12:L:89:ARG:NH2	12:L:97:ARG:HH21	2.19	0.40
18:R:21:LYS:O	18:R:22:VAL:C	2.58	0.40
19:S:62:ILE:CD1	19:S:66:MET:HG3	2.50	0.40
20:T:91:LEU:HD23	20:T:91:LEU:HA	1.85	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
2	B	233/256 (91%)	163 (70%)	49 (21%)	21 (9%)	1 1
3	C	205/239 (86%)	131 (64%)	50 (24%)	24 (12%)	0 1
4	D	206/209 (99%)	172 (84%)	27 (13%)	7 (3%)	3 15
5	E	149/162 (92%)	139 (93%)	9 (6%)	1 (1%)	22 54
6	F	99/101 (98%)	74 (75%)	22 (22%)	3 (3%)	4 17
7	G	153/156 (98%)	119 (78%)	26 (17%)	8 (5%)	2 6
8	H	136/138 (99%)	124 (91%)	10 (7%)	2 (2%)	10 34
9	I	125/128 (98%)	91 (73%)	22 (18%)	12 (10%)	0 1
10	J	97/105 (92%)	57 (59%)	28 (29%)	12 (12%)	0 1
11	K	117/129 (91%)	91 (78%)	20 (17%)	6 (5%)	2 7
12	L	123/135 (91%)	94 (76%)	19 (15%)	10 (8%)	1 2
13	M	123/126 (98%)	87 (71%)	24 (20%)	12 (10%)	0 1
14	N	58/61 (95%)	36 (62%)	14 (24%)	8 (14%)	0 0
15	O	86/89 (97%)	73 (85%)	13 (15%)	0	100 100
16	P	82/88 (93%)	71 (87%)	8 (10%)	3 (4%)	3 13
17	Q	102/105 (97%)	84 (82%)	10 (10%)	8 (8%)	1 2
18	R	71/88 (81%)	60 (84%)	7 (10%)	4 (6%)	2 5
19	S	79/93 (85%)	52 (66%)	17 (22%)	10 (13%)	0 0
20	T	97/106 (92%)	78 (80%)	10 (10%)	9 (9%)	0 1
21	U	23/27 (85%)	14 (61%)	8 (35%)	1 (4%)	2 10
All	All	2364/2541 (93%)	1810 (77%)	393 (17%)	161 (7%)	1 3

All (161) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	18	GLY
2	B	21	ARG
2	B	24	TRP
2	B	123	ALA
3	C	4	LYS
3	C	15	THR
3	C	16	ARG
3	C	26	LYS

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Mol	Chain	Res	Type
3	C	52	LEU
3	C	61	ALA
3	C	101	LEU
3	C	154	SER
3	C	179	ARG
3	C	205	GLY
4	D	3	ARG
4	D	36	ARG
8	H	83	ILE
8	H	91	ARG
9	I	7	THR
9	I	23	ASN
9	I	31	GLN
9	I	43	ALA
9	I	55	ALA
10	J	30	SER
10	J	34	VAL
10	J	39	PRO
10	J	54	PHE
10	J	90	LEU
11	K	12	ARG
12	L	27	LEU
12	L	41	ARG
12	L	47	LYS
13	M	23	TYR
13	M	24	GLY
13	M	63	THR
13	M	67	GLU
16	P	83	GLU
17	Q	80	GLY
17	Q	81	ARG
17	Q	97	SER
17	Q	98	LEU
18	R	20	ALA
18	R	87	ARG
19	S	6	LYS
19	S	9	VAL
19	S	81	ARG
20	T	74	LYS
2	B	20	GLU
2	B	95	GLN
2	B	119	GLU

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Mol	Chain	Res	Type
2	B	129	GLU
3	C	47	LEU
3	C	79	ARG
3	C	100	ALA
3	C	207	VAL
4	D	9	CYS
4	D	31	CYS
6	F	36	ARG
7	G	7	ALA
7	G	81	GLY
9	I	41	VAL
9	I	42	ARG
9	I	44	VAL
9	I	127	LYS
10	J	72	VAL
11	K	35	PRO
11	K	88	GLY
12	L	28	LYS
12	L	87	GLY
13	M	6	GLY
13	M	7	VAL
13	M	12	ASN
13	M	21	TYR
14	N	10	ALA
14	N	12	ARG
14	N	15	LYS
14	N	50	LYS
16	P	10	GLY
17	Q	75	ARG
18	R	22	VAL
19	S	68	GLY
20	T	96	GLY
20	T	102	GLY
21	U	3	LYS
2	B	74	LYS
2	B	191	ASP
3	C	27	LYS
3	C	156	ARG
4	D	4	TYR
6	F	72	VAL
7	G	53	LYS
10	J	40	LEU

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Mol	Chain	Res	Type
10	J	61	GLU
11	K	127	LYS
12	L	91	LYS
12	L	126	LYS
13	M	68	GLY
17	Q	69	LYS
17	Q	99	SER
19	S	43	GLU
20	T	11	SER
20	T	73	HIS
20	T	98	PRO
2	B	8	LYS
2	B	149	LEU
2	B	207	ALA
2	B	229	VAL
3	C	39	ILE
3	C	168	ALA
5	E	73	ASN
7	G	39	ALA
7	G	155	ARG
9	I	11	LYS
9	I	24	GLY
9	I	38	GLN
11	K	13	GLN
11	K	15	ALA
12	L	48	PRO
13	M	36	LYS
14	N	23	ARG
14	N	51	GLY
16	P	81	ARG
17	Q	96	GLN
18	R	26	LEU
19	S	3	ARG
20	T	46	GLU
20	T	95	ALA
2	B	63	MET
2	B	165	VAL
3	C	14	ILE
3	C	29	TYR
3	C	65	ALA
3	C	108	ASN
6	F	70	ASP

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Mol	Chain	Res	Type
7	G	56	GLN
7	G	153	HIS
10	J	6	ILE
10	J	33	GLN
10	J	76	ASN
14	N	13	THR
14	N	36	PHE
19	S	5	LEU
19	S	42	PRO
2	B	9	GLU
3	C	68	VAL
3	C	81	GLY
4	D	5	ILE
4	D	88	VAL
13	M	4	ILE
13	M	85	GLY
20	T	97	ALA
19	S	31	ILE
7	G	17	VAL
10	J	36	GLY
12	L	40	VAL
2	B	130	ARG
12	L	121	GLY
19	S	67	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
2	B	202/220 (92%)	187 (93%)	15 (7%)	13 38
3	C	160/188 (85%)	150 (94%)	10 (6%)	18 46
4	D	180/181 (99%)	167 (93%)	13 (7%)	14 39
5	E	115/123 (94%)	102 (89%)	13 (11%)	6 18
6	F	90/90 (100%)	85 (94%)	5 (6%)	21 52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	G	126/127 (99%)	119 (94%)	7 (6%)	21 52
8	H	119/119 (100%)	110 (92%)	9 (8%)	13 36
9	I	98/99 (99%)	89 (91%)	9 (9%)	9 27
10	J	87/92 (95%)	80 (92%)	7 (8%)	12 33
11	K	90/99 (91%)	87 (97%)	3 (3%)	38 72
12	L	104/111 (94%)	97 (93%)	7 (7%)	16 43
13	M	100/101 (99%)	92 (92%)	8 (8%)	12 33
14	N	49/50 (98%)	44 (90%)	5 (10%)	7 22
15	O	79/80 (99%)	71 (90%)	8 (10%)	7 23
16	P	72/74 (97%)	67 (93%)	5 (7%)	15 41
17	Q	96/97 (99%)	90 (94%)	6 (6%)	18 46
18	R	64/77 (83%)	59 (92%)	5 (8%)	12 34
19	S	71/80 (89%)	68 (96%)	3 (4%)	30 63
20	T	76/82 (93%)	69 (91%)	7 (9%)	9 27
21	U	19/22 (86%)	17 (90%)	2 (10%)	7 21
All	All	1997/2112 (95%)	1850 (93%)	147 (7%)	13 38

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	19	HIS
2	B	23	ARG
2	B	24	TRP
2	B	25	ASN
2	B	76	GLN
2	B	87	ARG
2	B	96	ARG
2	B	114	ARG
2	B	144	ARG
2	B	157	ARG
2	B	170	GLU
2	B	178	ARG
2	B	204	ASN
2	B	221	LEU
2	B	236	TYR
3	C	3	ASN
3	C	21	ARG

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Mol	Chain	Res	Type
3	C	26	LYS
3	C	37	GLN
3	C	88	ARG
3	C	167	TRP
3	C	179	ARG
3	C	190	ARG
3	C	192	THR
3	C	204	LEU
4	D	9	CYS
4	D	15	GLU
4	D	58	LEU
4	D	61	LYS
4	D	65	ARG
4	D	122	ARG
4	D	157	LEU
4	D	162	LEU
4	D	170	VAL
4	D	177	ASP
4	D	192	GLU
4	D	199	ASN
4	D	201	GLN
5	E	12	LEU
5	E	31	LEU
5	E	41	VAL
5	E	43	LEU
5	E	64	ARG
5	E	73	ASN
5	E	79	GLU
5	E	80	ILE
5	E	89	ILE
5	E	116	THR
5	E	120	THR
5	E	144	THR
5	E	151	LEU
6	F	1	MET
6	F	47	ARG
6	F	82	ARG
6	F	95	GLU
6	F	100	ASN
7	G	4	ARG
7	G	8	GLU
7	G	12	LEU

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Mol	Chain	Res	Type
7	G	114	ARG
7	G	136	LYS
7	G	140	ASP
7	G	156	TRP
8	H	39	LEU
8	H	56	LYS
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	97	VAL
8	H	105	ARG
8	H	112	LEU
8	H	133	LEU
9	I	2	GLU
9	I	23	ASN
9	I	38	GLN
9	I	79	LEU
9	I	111	ARG
9	I	113	LYS
9	I	116	LYS
9	I	118	LYS
9	I	121	ARG
10	J	57	LYS
10	J	58	ASP
10	J	65	LEU
10	J	71	LEU
10	J	73	ASP
10	J	83	GLU
10	J	98	ILE
11	K	29	ILE
11	K	35	PRO
11	K	54	ARG
12	L	17	LYS
12	L	48	PRO
12	L	59	ARG
12	L	60	LEU
12	L	93	LEU
12	L	113	ARG
12	L	126	LYS
13	M	9	ILE
13	M	16	ASP
13	M	40	ASN

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Mol	Chain	Res	Type
13	M	70	LEU
13	M	81	LEU
13	M	110	ARG
13	M	115	LYS
13	M	125	ARG
14	N	3	ARG
14	N	14	PRO
14	N	22	THR
14	N	27	CYS
14	N	52	GLN
15	O	13	GLN
15	O	17	ARG
15	O	31	LEU
15	O	34	LEU
15	O	40	SER
15	O	64	ARG
15	O	70	LEU
15	O	81	LEU
16	P	1	MET
16	P	2	VAL
16	P	8	ARG
16	P	28	ARG
16	P	53	VAL
17	Q	34	LYS
17	Q	38	ARG
17	Q	60	ILE
17	Q	92	ARG
17	Q	98	LEU
17	Q	101	ARG
18	R	19	LYS
18	R	28	GLU
18	R	36	ASN
18	R	54	ARG
18	R	87	ARG
19	S	15	LEU
19	S	42	PRO
19	S	65	ASN
20	T	10	LEU
20	T	13	LEU
20	T	24	LEU
20	T	42	GLN
20	T	57	ARG

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Mol	Chain	Res	Type
20	T	75	ASN
20	T	84	LEU
21	U	6	ARG
21	U	24	ARG

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

Mol	Chain	Res	Type
2	B	25	ASN
2	B	76	GLN
2	B	78	GLN
2	B	140	HIS
2	B	146	GLN
2	B	204	ASN
2	B	240	GLN
3	C	3	ASN
3	C	6	HIS
3	C	31	HIS
3	C	37	GLN
3	C	69	HIS
3	C	102	ASN
3	C	107	GLN
3	C	108	ASN
3	C	118	GLN
3	C	123	GLN
3	C	139	GLN
3	C	170	GLN
4	D	42	GLN
4	D	62	GLN
4	D	119	GLN
4	D	160	GLN
4	D	161	ASN
4	D	199	ASN
5	E	73	ASN
6	F	18	GLN
6	F	27	GLN
6	F	32	ASN
6	F	57	GLN
6	F	73	ASN
6	F	94	GLN
6	F	100	ASN
7	G	37	ASN

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Mol	Chain	Res	Type
7	G	68	ASN
7	G	86	GLN
7	G	106	GLN
8	H	82	HIS
9	I	23	ASN
9	I	73	GLN
10	J	56	HIS
10	J	62	HIS
10	J	76	ASN
10	J	78	ASN
10	J	84	GLN
11	K	13	GLN
11	K	38	ASN
11	K	93	GLN
11	K	117	ASN
12	L	49	ASN
12	L	75	HIS
13	M	12	ASN
13	M	40	ASN
13	M	62	ASN
15	O	13	GLN
15	O	37	ASN
16	P	76	GLN
16	P	82	GLN
17	Q	94	ASN
18	R	36	ASN
19	S	14	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1522 (99%)	222 (14%)	75 (4%)
22	X	8/18 (44%)	2 (25%)	0
23	Y	3/5 (60%)	1 (33%)	0
All	All	1524/1545 (98%)	225 (14%)	75 (4%)

All (225) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A

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Mol	Chain	Res	Type
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	52	G
1	A	61	G
1	A	81	U
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	182	U
1	A	190(D)	U
1	A	190(E)	U
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	280	C
1	A	282	A
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	345	C
1	A	352	C
1	A	353	A

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Mol	Chain	Res	Type
1	A	354	G
1	A	367	U
1	A	373	A
1	A	397	A
1	A	398	C
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	415	A
1	A	421	U
1	A	424	G
1	A	429	U
1	A	430	A
1	A	432	A
1	A	434	U
1	A	439	A
1	A	443	C
1	A	444	C
1	A	452	A
1	A	461	C
1	A	462	G
1	A	476	G
1	A	478	A
1	A	479	C
1	A	484	G
1	A	485	G
1	A	486	U
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	G
1	A	531	U
1	A	533	A
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	U

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Mol	Chain	Res	Type
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	588	G
1	A	653	A
1	A	661	G
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	702	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	733	A
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	965	A
1	A	966	G
1	A	969	A

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Mol	Chain	Res	Type
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1023	G
1	A	1026	G
1	A	1045	C
1	A	1050	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1070	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1117	G
1	A	1126	U
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1183	A
1	A	1184	G
1	A	1196	U
1	A	1197	G
1	A	1200	C

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Mol	Chain	Res	Type
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1238	A
1	A	1257	U
1	A	1278	U
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1320	C
1	A	1332	A
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1379	G
1	A	1381	U
1	A	1398	A
1	A	1442	G
1	A	1446	A
1	A	1447	G
1	A	1452	C
1	A	1492	A
1	A	1497	G
1	A	1498	U
1	A	1499	A
1	A	1502	A
1	A	1504	G

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Mol	Chain	Res	Type
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1534	A
1	A	1539	C
22	X	41	C
22	X	42	U
23	Y	4	U

All (75) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	7	G
1	A	30	U
1	A	51	A
1	A	60	A
1	A	81	U
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	202	U
1	A	243	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	279	A
1	A	281	G
1	A	328	C
1	A	344	A
1	A	351	G
1	A	353	A
1	A	366	C
1	A	372	C
1	A	428	G
1	A	429	U

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Mol	Chain	Res	Type
1	A	484	G
1	A	485	G
1	A	496	A
1	A	497	A
1	A	509	A
1	A	533	A
1	A	559	A
1	A	560	U
1	A	575	G
1	A	687	A
1	A	701	C
1	A	792	A
1	A	793	U
1	A	812	C
1	A	819	A
1	A	840	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	975	A
1	A	992	U
1	A	993	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1101	A
1	A	1129	C
1	A	1145	C
1	A	1182	G
1	A	1183	A
1	A	1196	U
1	A	1201	A
1	A	1224	G
1	A	1226	C
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1331	G
1	A	1346	A
1	A	1347	G

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Mol	Chain	Res	Type
1	A	1380	U
1	A	1397	C
1	A	1451	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1528	U

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 221 ligands modelled in this entry, 220 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	$\#\|Z\| > 2$
24	PAR	A	2001	-	45,45,45	1.57	8 (17%)	64,67,67	1.31	8 (12%)

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
24	PAR	A	2001	-	-	4/18/94/94	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	2001	PAR	C64-C54	5.52	1.59	1.52
24	A	2001	PAR	O54-C14	3.32	1.50	1.41
24	A	2001	PAR	C52-C42	2.82	1.58	1.52
24	A	2001	PAR	C14-C24	2.57	1.57	1.52
24	A	2001	PAR	C31-C21	2.36	1.56	1.53
24	A	2001	PAR	C11-C21	2.30	1.56	1.52
24	A	2001	PAR	O51-C11	2.15	1.47	1.41
24	A	2001	PAR	O54-C54	2.04	1.49	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	2001	PAR	O33-C14-C24	5.03	116.88	108.22
24	A	2001	PAR	C14-O54-C54	3.80	121.15	113.69
24	A	2001	PAR	O54-C54-C64	3.64	112.79	106.01
24	A	2001	PAR	O52-C13-C23	3.20	114.59	107.96
24	A	2001	PAR	O52-C13-O43	-2.46	108.77	111.43
24	A	2001	PAR	C11-O51-C51	2.10	117.81	113.69
24	A	2001	PAR	O11-C11-C21	2.03	111.71	108.22
24	A	2001	PAR	C22-C32-C42	2.02	114.63	109.53

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	2001	PAR	C44-C54-C64-N64
24	A	2001	PAR	C23-C13-O52-C52
24	A	2001	PAR	C23-C33-O33-C14
24	A	2001	PAR	C43-C33-O33-C14

There are no ring outliers.

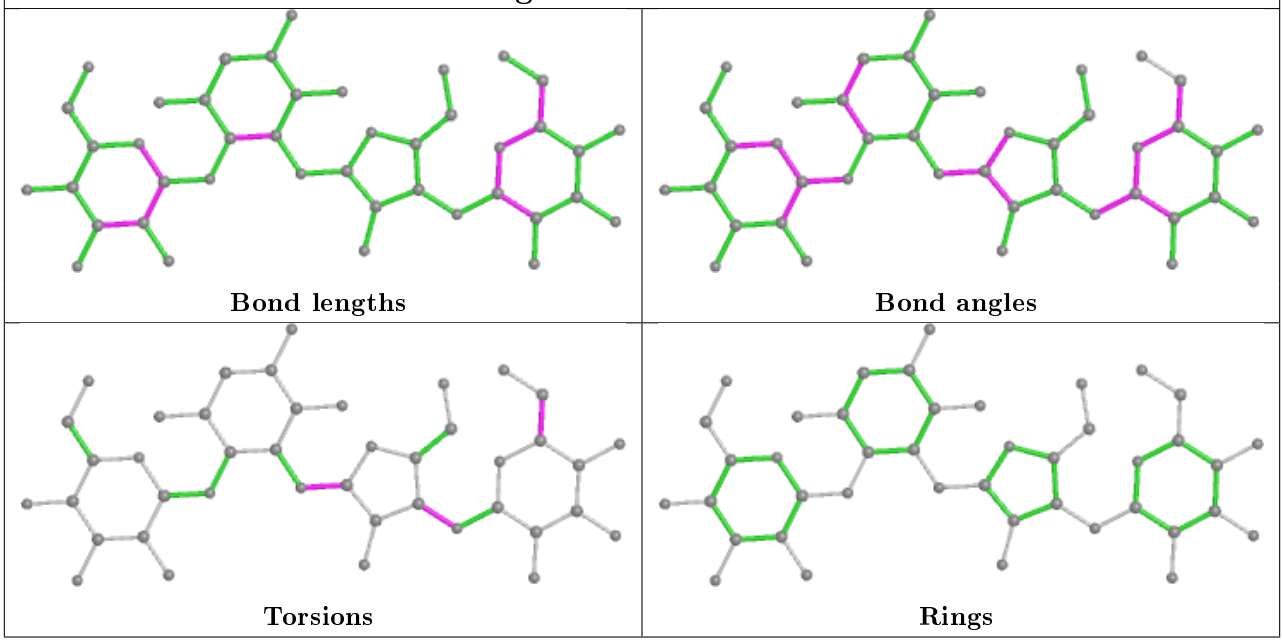
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	2001	PAR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

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

Ligand PAR A 2001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1513/1522 (99%)	0.40	60 (3%) 38 33	33, 64, 141, 201	0
2	B	235/256 (91%)	0.32	17 (7%) 15 11	45, 97, 164, 200	0
3	C	207/239 (86%)	0.36	12 (5%) 23 19	47, 91, 150, 185	0
4	D	208/209 (99%)	0.16	11 (5%) 26 22	43, 74, 123, 200	0
5	E	151/162 (93%)	-0.09	0 100 100	34, 55, 93, 201	0
6	F	101/101 (100%)	0.12	1 (0%) 82 82	57, 92, 120, 147	0
7	G	155/156 (99%)	0.05	5 (3%) 47 43	48, 83, 148, 200	0
8	H	138/138 (100%)	-0.27	0 100 100	30, 51, 80, 144	0
9	I	127/128 (99%)	0.56	9 (7%) 16 12	40, 98, 131, 158	0
10	J	99/105 (94%)	1.09	17 (17%) 1 1	44, 119, 194, 201	0
11	K	119/129 (92%)	0.00	1 (0%) 86 86	33, 67, 109, 171	0
12	L	125/135 (92%)	0.07	2 (1%) 72 71	21, 67, 111, 175	0
13	M	125/126 (99%)	0.96	14 (11%) 5 4	55, 81, 157, 199	0
14	N	60/61 (98%)	0.17	0 100 100	54, 85, 117, 191	0
15	O	88/89 (98%)	-0.11	1 (1%) 80 80	39, 66, 109, 187	0
16	P	84/88 (95%)	-0.09	0 100 100	33, 54, 96, 146	0
17	Q	104/105 (99%)	0.25	6 (5%) 23 19	30, 56, 127, 201	0
18	R	73/88 (82%)	0.21	4 (5%) 25 21	48, 76, 160, 181	0
19	S	81/93 (87%)	0.58	8 (9%) 7 5	68, 105, 147, 201	0
20	T	99/106 (93%)	0.07	2 (2%) 65 63	33, 64, 107, 128	0
21	U	25/27 (92%)	0.24	0 100 100	43, 68, 114, 156	0
22	X	9/18 (50%)	1.17	2 (22%) 0 0	72, 94, 173, 190	0
23	Y	5/5 (100%)	1.02	1 (20%) 1 0	80, 81, 145, 171	0
All	All	3931/4086 (96%)	0.30	173 (4%) 34 30	21, 72, 143, 201	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	123	ALA	27.0
1	A	1534	A	23.4
13	M	124	PRO	20.1
17	Q	102	GLY	13.5
13	M	125	ARG	13.4
1	A	415	A	10.7
13	M	120	LYS	8.3
1	A	432	A	8.1
13	M	122	LYS	8.1
1	A	1129	C	7.9
17	Q	105	ALA	7.7
4	D	23	GLY	7.3
19	S	3	ARG	6.2
1	A	1539	C	6.0
13	M	121	LYS	5.8
9	I	128	ARG	5.7
10	J	34	VAL	5.6
10	J	24	VAL	5.6
15	O	89	GLY	5.5
1	A	416	G	5.5
1	A	417	C	5.4
1	A	1006	C	5.4
13	M	126	LYS	5.4
10	J	90	LEU	5.1
1	A	412	A	5.0
17	Q	103	GLY	4.9
13	M	7	VAL	4.9
17	Q	104	LYS	4.8
17	Q	101	ARG	4.8
1	A	418	C	4.8
18	R	16	PRO	4.7
10	J	10	GLY	4.7
2	B	16	HIS	4.7
9	I	17	VAL	4.7
1	A	1005	A	4.5
7	G	156	TRP	4.4
1	A	1257	U	4.4
10	J	33	GLN	4.3
13	M	6	GLY	4.3
1	A	443	C	4.3
1	A	1004	A	4.2
18	R	17	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1540	U	4.0
13	M	117	VAL	4.0
17	Q	96	GLN	3.9
10	J	99	LYS	3.9
13	M	119	GLY	3.9
1	A	1024	G	3.8
1	A	1533	C	3.7
11	K	128	ALA	3.7
9	I	92	TYR	3.7
1	A	1003(A)	G	3.7
22	X	41	C	3.5
4	D	36	ARG	3.5
1	A	1478	C	3.5
19	S	29	ARG	3.4
2	B	238	LEU	3.4
18	R	18	ARG	3.4
1	A	1038	C	3.4
9	I	96	LEU	3.3
1	A	1034	G	3.3
3	C	60	ALA	3.3
1	A	1026	G	3.3
1	A	1027	C	3.2
10	J	35	SER	3.2
2	B	231	GLU	3.2
1	A	1144	G	3.1
1	A	1036	G	3.1
10	J	87	THR	3.1
10	J	72	VAL	3.0
13	M	8	GLU	3.0
1	A	993	G	3.0
1	A	1001	A	2.9
7	G	5	ARG	2.9
1	A	1023	G	2.9
1	A	413	G	2.9
2	B	209	ARG	2.9
1	A	1025	U	2.9
3	C	65	ALA	2.9
12	L	50	SER	2.8
1	A	532	A	2.8
9	I	19	LEU	2.8
1	A	1007	C	2.8
3	C	178	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	723	U	2.8
4	D	35	ARG	2.8
1	A	1138	G	2.8
3	C	64	VAL	2.8
2	B	132	LYS	2.8
2	B	208	ILE	2.7
1	A	1140	C	2.7
10	J	85	LEU	2.7
19	S	34	TRP	2.7
4	D	4	TYR	2.7
3	C	102	ASN	2.7
10	J	76	ASN	2.7
23	Y	5	U	2.7
2	B	19	HIS	2.7
3	C	66	VAL	2.7
2	B	36	ARG	2.7
13	M	116	THR	2.7
13	M	118	ALA	2.6
1	A	1003	G	2.6
10	J	6	ILE	2.6
1	A	1541	U	2.6
1	A	1002	G	2.6
1	A	1035	A	2.6
1	A	1124	G	2.6
1	A	1477	C	2.6
2	B	130	ARG	2.6
2	B	211	ILE	2.6
1	A	992	U	2.6
1	A	1143	G	2.6
7	G	2	ALA	2.6
2	B	229	VAL	2.5
6	F	61	LEU	2.5
9	I	102	LEU	2.5
9	I	6	GLY	2.5
2	B	237	ALA	2.5
1	A	1446	A	2.4
4	D	209	ARG	2.4
1	A	1476	G	2.4
2	B	125	PRO	2.4
1	A	841	U	2.4
4	D	9	CYS	2.4
1	A	991	U	2.4

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Mol	Chain	Res	Type	RSRZ
10	J	83	GLU	2.4
4	D	26	CYS	2.4
4	D	37	PRO	2.4
19	S	31	ILE	2.4
1	A	1278	U	2.4
4	D	29	PRO	2.3
3	C	76	VAL	2.3
10	J	5	ARG	2.3
4	D	32	ALA	2.3
3	C	188	LEU	2.3
1	A	1137	C	2.3
3	C	101	LEU	2.3
19	S	54	GLY	2.3
20	T	103	GLY	2.3
2	B	131	PRO	2.3
1	A	1019	C	2.2
7	G	143	ARG	2.2
1	A	411	A	2.2
2	B	40	HIS	2.2
2	B	122	PHE	2.2
9	I	15	ALA	2.2
1	A	1132	C	2.2
9	I	33	PHE	2.2
10	J	4	ILE	2.2
7	G	56	GLN	2.2
1	A	1033	G	2.2
1	A	1008	C	2.2
1	A	1032	G	2.2
1	A	1135	U	2.2
19	S	49	ILE	2.1
3	C	78	GLY	2.1
22	X	42	U	2.1
10	J	70	ARG	2.1
1	A	1274	G	2.1
18	R	25	THR	2.1
1	A	1276	G	2.1
2	B	35	GLU	2.1
3	C	103	VAL	2.1
1	A	1126	U	2.1
3	C	68	VAL	2.1
4	D	25	ARG	2.1
19	S	28	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1031	G	2.1
10	J	9	ARG	2.0
19	S	16	LEU	2.0
12	L	28	LYS	2.0
20	T	74	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	2087	1/1	0.54	0.27	51,51,51,51	0
25	MG	A	2080	1/1	0.58	0.20	51,51,51,51	0
25	MG	A	2138	1/1	0.58	0.29	51,51,51,51	1
25	MG	A	2077	1/1	0.61	0.27	51,51,51,51	1
25	MG	A	2146	1/1	0.65	0.22	51,51,51,51	1
26	K	A	2205	1/1	0.66	0.19	51,51,51,51	1
25	MG	A	2125	1/1	0.66	0.55	51,51,51,51	0
25	MG	A	2025	1/1	0.67	0.46	51,51,51,51	0
25	MG	A	2184	1/1	0.69	0.45	51,51,51,51	0
25	MG	A	2076	1/1	0.69	0.25	51,51,51,51	0
25	MG	A	2047	1/1	0.72	0.23	51,51,51,51	1
26	K	A	2217	1/1	0.72	0.20	51,51,51,51	1
25	MG	A	2130	1/1	0.73	0.36	51,51,51,51	0
25	MG	A	2046	1/1	0.73	0.32	51,51,51,51	0
25	MG	A	2148	1/1	0.74	0.42	51,51,51,51	1
25	MG	A	2164	1/1	0.74	0.22	51,51,51,51	1
25	MG	A	2183	1/1	0.75	0.14	51,51,51,51	0
25	MG	A	2140	1/1	0.75	0.22	51,51,51,51	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	2141	1/1	0.76	0.20	51,51,51,51	1
25	MG	A	2131	1/1	0.76	0.18	51,51,51,51	1
25	MG	A	2105	1/1	0.76	0.33	51,51,51,51	0
25	MG	A	2078	1/1	0.76	0.21	51,51,51,51	0
25	MG	A	2119	1/1	0.77	0.16	51,51,51,51	0
25	MG	A	2124	1/1	0.78	0.31	51,51,51,51	0
26	K	A	2218	1/1	0.79	0.23	51,51,51,51	1
25	MG	A	2102	1/1	0.79	0.21	51,51,51,51	0
25	MG	A	2122	1/1	0.80	0.29	51,51,51,51	1
25	MG	A	2023	1/1	0.80	0.53	51,51,51,51	0
25	MG	A	2116	1/1	0.80	0.10	51,51,51,51	0
25	MG	A	2161	1/1	0.80	0.26	51,51,51,51	1
25	MG	A	2166	1/1	0.81	0.42	51,51,51,51	0
25	MG	A	2151	1/1	0.81	0.25	51,51,51,51	0
25	MG	A	2081	1/1	0.81	0.25	51,51,51,51	0
25	MG	A	2139	1/1	0.82	0.22	51,51,51,51	0
25	MG	A	2003	1/1	0.82	0.23	51,51,51,51	0
25	MG	A	2126	1/1	0.82	0.19	51,51,51,51	1
25	MG	A	2088	1/1	0.82	0.47	51,51,51,51	0
25	MG	A	2083	1/1	0.82	0.22	51,51,51,51	1
25	MG	A	2178	1/1	0.83	0.19	51,51,51,51	0
25	MG	A	2036	1/1	0.83	0.20	51,51,51,51	1
25	MG	A	2050	1/1	0.83	0.22	51,51,51,51	0
25	MG	A	2065	1/1	0.83	0.26	51,51,51,51	0
25	MG	A	2070	1/1	0.83	0.09	51,51,51,51	0
25	MG	A	2022	1/1	0.84	0.47	51,51,51,51	0
25	MG	A	2101	1/1	0.84	0.23	51,51,51,51	1
25	MG	A	2157	1/1	0.84	0.25	51,51,51,51	0
25	MG	A	2174	1/1	0.85	0.10	51,51,51,51	0
25	MG	A	2055	1/1	0.85	0.26	51,51,51,51	0
25	MG	A	2093	1/1	0.85	0.35	51,51,51,51	1
25	MG	A	2004	1/1	0.86	0.28	51,51,51,51	0
25	MG	A	2062	1/1	0.86	0.25	51,51,51,51	0
25	MG	A	2144	1/1	0.86	0.25	51,51,51,51	0
25	MG	A	2177	1/1	0.86	0.39	51,51,51,51	0
25	MG	A	2114	1/1	0.86	0.42	51,51,51,51	1
25	MG	A	2021	1/1	0.86	0.35	51,51,51,51	0
26	K	A	2216	1/1	0.86	0.44	51,51,51,51	1
25	MG	A	2172	1/1	0.86	0.17	51,51,51,51	0
25	MG	A	2179	1/1	0.86	0.44	51,51,51,51	0
25	MG	A	2103	1/1	0.87	0.14	51,51,51,51	1
25	MG	A	2097	1/1	0.87	0.21	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	K	A	2209	1/1	0.87	0.20	51,51,51,51	0
25	MG	A	2090	1/1	0.87	0.17	51,51,51,51	1
25	MG	A	2061	1/1	0.87	0.60	51,51,51,51	0
25	MG	A	2188	1/1	0.87	0.07	51,51,51,51	1
26	K	A	2202	1/1	0.87	0.26	51,51,51,51	1
25	MG	A	2121	1/1	0.87	0.49	51,51,51,51	0
25	MG	A	2042	1/1	0.87	0.50	51,51,51,51	0
25	MG	A	2086	1/1	0.87	0.78	51,51,51,51	0
25	MG	A	2120	1/1	0.87	0.15	51,51,51,51	1
25	MG	A	2156	1/1	0.87	0.12	51,51,51,51	0
25	MG	A	2176	1/1	0.88	0.14	51,51,51,51	0
25	MG	A	2154	1/1	0.88	0.47	51,51,51,51	0
25	MG	A	2098	1/1	0.88	0.27	51,51,51,51	0
25	MG	A	2111	1/1	0.88	0.21	51,51,51,51	1
25	MG	A	2058	1/1	0.88	0.13	51,51,51,51	0
25	MG	A	2104	1/1	0.88	0.23	51,51,51,51	0
25	MG	A	2159	1/1	0.88	0.30	51,51,51,51	1
25	MG	A	2045	1/1	0.89	0.27	51,51,51,51	0
25	MG	A	2182	1/1	0.89	0.16	51,51,51,51	0
25	MG	A	2145	1/1	0.89	0.11	51,51,51,51	0
25	MG	A	2064	1/1	0.89	0.38	51,51,51,51	0
25	MG	A	2031	1/1	0.89	0.38	51,51,51,51	0
25	MG	A	2187	1/1	0.89	0.13	51,51,51,51	0
25	MG	A	2048	1/1	0.89	0.24	51,51,51,51	0
25	MG	A	2043	1/1	0.89	0.21	51,51,51,51	0
25	MG	A	2149	1/1	0.89	0.42	51,51,51,51	0
25	MG	A	2191	1/1	0.89	0.82	51,51,51,51	0
25	MG	A	2167	1/1	0.89	0.37	51,51,51,51	0
25	MG	A	2127	1/1	0.90	0.35	51,51,51,51	0
26	K	A	2212	1/1	0.90	0.09	51,51,51,51	1
25	MG	A	2052	1/1	0.90	0.32	51,51,51,51	0
25	MG	A	2142	1/1	0.90	0.46	51,51,51,51	0
25	MG	A	2005	1/1	0.90	0.65	51,51,51,51	0
26	K	A	2213	1/1	0.90	0.16	51,51,51,51	1
25	MG	A	2129	1/1	0.90	0.53	51,51,51,51	0
26	K	A	2208	1/1	0.90	0.30	51,51,51,51	1
25	MG	A	2011	1/1	0.90	0.64	51,51,51,51	0
25	MG	A	2189	1/1	0.90	0.28	51,51,51,51	0
25	MG	A	2059	1/1	0.90	0.69	51,51,51,51	0
25	MG	A	2071	1/1	0.90	0.29	51,51,51,51	0
25	MG	A	2169	1/1	0.91	0.30	51,51,51,51	0
25	MG	A	2170	1/1	0.91	0.09	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	2009	1/1	0.91	0.36	51,51,51,51	0
25	MG	A	2060	1/1	0.91	0.66	51,51,51,51	0
25	MG	A	2069	1/1	0.91	0.26	51,51,51,51	0
25	MG	A	2053	1/1	0.91	0.62	51,51,51,51	0
26	K	A	2215	1/1	0.91	0.32	51,51,51,51	1
25	MG	A	2072	1/1	0.91	0.60	51,51,51,51	0
25	MG	A	2185	1/1	0.91	0.20	51,51,51,51	0
25	MG	A	2155	1/1	0.91	0.38	51,51,51,51	1
25	MG	A	2181	1/1	0.91	0.23	51,51,51,51	0
25	MG	A	2110	1/1	0.91	0.40	51,51,51,51	0
25	MG	A	2158	1/1	0.91	0.27	51,51,51,51	0
25	MG	A	2019	1/1	0.91	0.57	51,51,51,51	0
24	PAR	A	2001	42/42	0.92	0.28	78,78,78,78	0
25	MG	A	2136	1/1	0.92	1.11	51,51,51,51	0
25	MG	A	2095	1/1	0.92	0.15	51,51,51,51	0
25	MG	A	2014	1/1	0.92	0.27	51,51,51,51	0
25	MG	A	2099	1/1	0.92	0.08	51,51,51,51	0
25	MG	A	2112	1/1	0.92	0.25	51,51,51,51	0
25	MG	A	2054	1/1	0.92	0.43	51,51,51,51	0
25	MG	A	2039	1/1	0.92	0.33	51,51,51,51	0
25	MG	A	2020	1/1	0.92	0.22	51,51,51,51	0
26	K	A	2199	1/1	0.92	0.14	51,51,51,51	1
26	K	A	2201	1/1	0.92	0.32	51,51,51,51	1
25	MG	A	2089	1/1	0.92	0.38	51,51,51,51	0
25	MG	A	2015	1/1	0.93	0.65	51,51,51,51	0
25	MG	A	2044	1/1	0.93	0.35	51,51,51,51	0
25	MG	A	2018	1/1	0.93	0.61	51,51,51,51	0
25	MG	A	2162	1/1	0.93	0.17	51,51,51,51	1
25	MG	A	2128	1/1	0.93	0.11	51,51,51,51	0
25	MG	A	2056	1/1	0.93	0.57	51,51,51,51	0
25	MG	A	2017	1/1	0.93	0.19	51,51,51,51	0
26	K	A	2207	1/1	0.93	0.26	51,51,51,51	1
25	MG	A	2067	1/1	0.93	0.34	51,51,51,51	0
25	MG	A	2175	1/1	0.93	0.46	51,51,51,51	0
25	MG	A	2134	1/1	0.93	0.19	51,51,51,51	1
25	MG	A	2168	1/1	0.93	0.26	51,51,51,51	0
25	MG	A	2163	1/1	0.93	0.27	51,51,51,51	0
25	MG	A	2041	1/1	0.93	0.41	51,51,51,51	0
26	K	A	2198	1/1	0.93	0.18	51,51,51,51	1
25	MG	A	2152	1/1	0.93	0.41	51,51,51,51	0
25	MG	A	2153	1/1	0.94	0.26	51,51,51,51	0
25	MG	A	2106	1/1	0.94	0.49	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	2115	1/1	0.94	0.64	51,51,51,51	0
25	MG	A	2171	1/1	0.94	0.14	51,51,51,51	0
25	MG	A	2024	1/1	0.94	0.78	51,51,51,51	0
25	MG	A	2068	1/1	0.94	0.34	51,51,51,51	0
25	MG	A	2008	1/1	0.94	0.53	51,51,51,51	0
25	MG	A	2117	1/1	0.94	0.55	51,51,51,51	0
25	MG	A	2193	1/1	0.94	0.43	51,51,51,51	0
25	MG	A	2165	1/1	0.94	0.22	51,51,51,51	1
25	MG	A	2027	1/1	0.94	0.51	51,51,51,51	0
25	MG	A	2160	1/1	0.94	0.25	51,51,51,51	0
25	MG	A	2066	1/1	0.94	0.18	51,51,51,51	0
25	MG	A	2173	1/1	0.94	0.23	51,51,51,51	0
26	K	A	2200	1/1	0.94	0.22	51,51,51,51	1
25	MG	A	2035	1/1	0.94	0.40	51,51,51,51	0
26	K	A	2214	1/1	0.94	0.11	51,51,51,51	1
25	MG	A	2026	1/1	0.94	0.64	51,51,51,51	0
25	MG	A	2032	1/1	0.94	0.33	51,51,51,51	0
25	MG	A	2085	1/1	0.94	0.23	51,51,51,51	0
25	MG	A	2192	1/1	0.94	0.20	51,51,51,51	0
25	MG	A	2123	1/1	0.94	0.10	51,51,51,51	0
25	MG	A	2108	1/1	0.94	0.33	51,51,51,51	0
26	K	A	2211	1/1	0.94	0.26	51,51,51,51	1
26	K	A	2204	1/1	0.94	0.18	51,51,51,51	1
25	MG	A	2118	1/1	0.94	0.45	51,51,51,51	0
25	MG	A	2107	1/1	0.95	0.17	51,51,51,51	0
26	K	A	2210	1/1	0.95	0.18	51,51,51,51	1
25	MG	A	2006	1/1	0.95	0.18	51,51,51,51	0
26	K	A	2196	1/1	0.95	0.20	51,51,51,51	1
25	MG	A	2075	1/1	0.95	0.15	51,51,51,51	0
25	MG	A	2100	1/1	0.95	0.10	51,51,51,51	0
26	K	A	2195	1/1	0.95	0.22	51,51,51,51	1
25	MG	A	2190	1/1	0.95	0.09	51,51,51,51	0
25	MG	A	2096	1/1	0.95	0.39	51,51,51,51	0
26	K	A	2197	1/1	0.95	0.22	51,51,51,51	1
25	MG	A	2040	1/1	0.95	0.44	51,51,51,51	0
25	MG	A	2135	1/1	0.95	0.13	51,51,51,51	0
25	MG	A	2180	1/1	0.96	0.11	51,51,51,51	0
25	MG	A	2030	1/1	0.96	0.76	51,51,51,51	0
25	MG	A	2137	1/1	0.96	0.32	51,51,51,51	0
25	MG	A	2147	1/1	0.96	0.42	51,51,51,51	0
25	MG	A	2073	1/1	0.96	0.47	51,51,51,51	0
25	MG	A	2016	1/1	0.96	0.52	51,51,51,51	0

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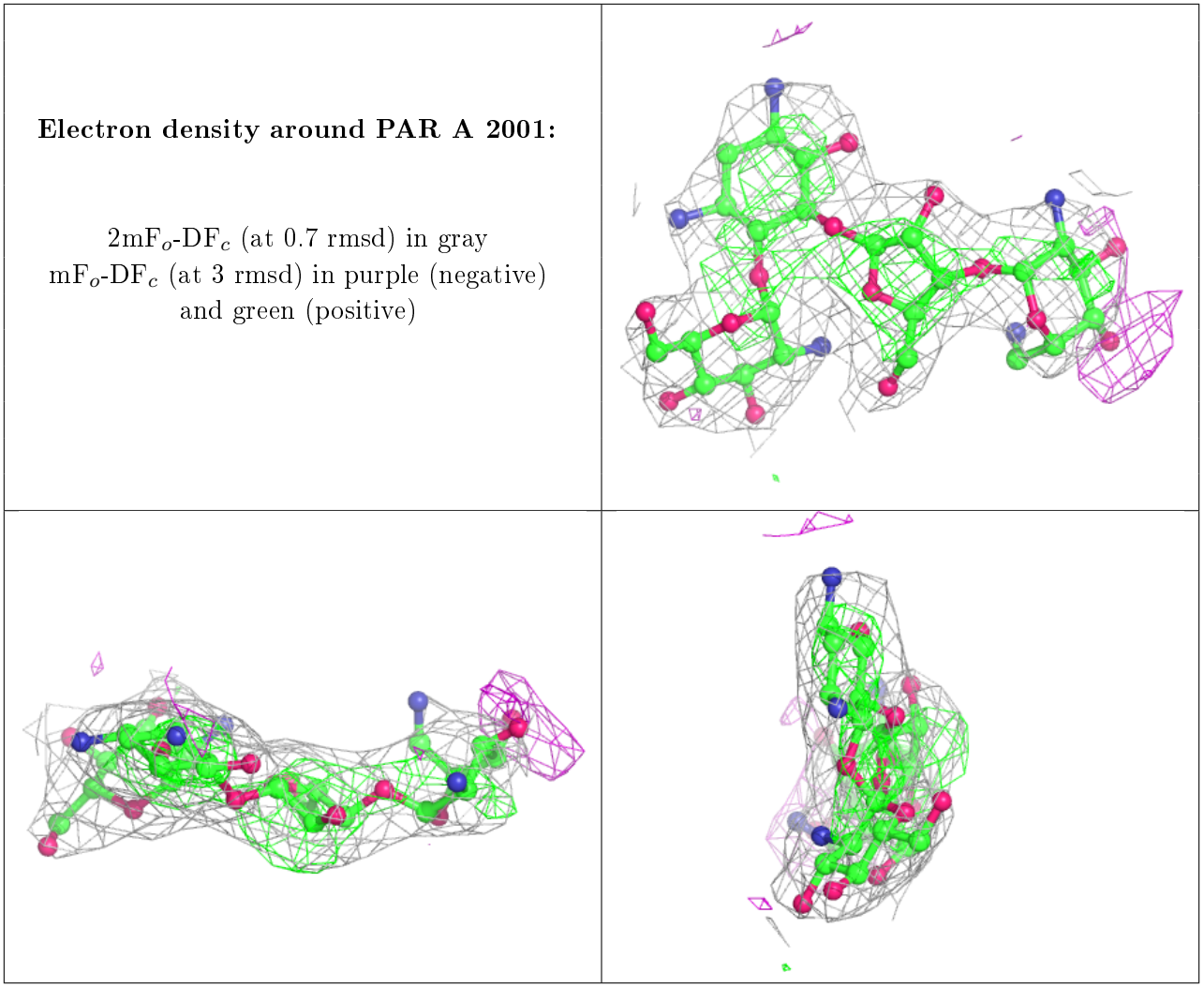
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	2109	1/1	0.96	0.16	51,51,51,51	0
25	MG	A	2002	1/1	0.96	0.59	51,51,51,51	0
25	MG	A	2132	1/1	0.96	0.66	51,51,51,51	0
25	MG	A	2094	1/1	0.96	0.10	51,51,51,51	0
25	MG	A	2074	1/1	0.96	0.42	51,51,51,51	0
25	MG	A	2038	1/1	0.96	0.39	51,51,51,51	0
25	MG	A	2037	1/1	0.96	0.46	51,51,51,51	0
25	MG	A	2150	1/1	0.96	0.44	51,51,51,51	0
25	MG	A	2143	1/1	0.96	0.21	51,51,51,51	1
25	MG	A	2033	1/1	0.96	0.24	51,51,51,51	0
25	MG	A	2034	1/1	0.96	0.90	51,51,51,51	0
25	MG	A	2010	1/1	0.97	0.47	51,51,51,51	0
25	MG	A	2082	1/1	0.97	0.72	51,51,51,51	0
27	ZN	A	2220	1/1	0.97	0.24	51,51,51,51	0
26	K	A	2206	1/1	0.97	0.10	51,51,51,51	1
25	MG	A	2057	1/1	0.97	0.51	51,51,51,51	0
25	MG	A	2084	1/1	0.97	0.23	51,51,51,51	0
25	MG	A	2133	1/1	0.97	0.09	51,51,51,51	0
25	MG	A	2028	1/1	0.97	0.25	51,51,51,51	0
25	MG	A	2092	1/1	0.97	0.58	51,51,51,51	0
25	MG	A	2029	1/1	0.97	0.44	51,51,51,51	0
25	MG	A	2186	1/1	0.98	0.24	51,51,51,51	0
25	MG	A	2063	1/1	0.98	0.54	51,51,51,51	0
25	MG	A	2007	1/1	0.98	0.51	51,51,51,51	0
25	MG	A	2079	1/1	0.98	0.52	51,51,51,51	0
25	MG	A	2012	1/1	0.98	0.50	51,51,51,51	0
25	MG	A	2051	1/1	0.98	0.57	51,51,51,51	0
26	K	A	2194	1/1	0.98	0.10	51,51,51,51	1
25	MG	A	2013	1/1	0.98	0.45	51,51,51,51	0
26	K	A	2203	1/1	0.98	0.08	51,51,51,51	1
26	K	A	2219	1/1	0.98	0.42	51,51,51,51	1
25	MG	A	2049	1/1	0.99	0.05	51,51,51,51	0
25	MG	A	2091	1/1	0.99	0.12	51,51,51,51	1
27	ZN	A	2221	1/1	0.99	0.16	51,51,51,51	1
25	MG	A	2113	1/1	0.99	0.16	51,51,51,51	0

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

Electron density around PAR A 2001:

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



6.5 Other polymers

There are no such residues in this entry.