Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 05:57 AM EDT

PDB ID	:	2UXD
Title	:	Crystal structure of an extended tRNA anticodon stem loop in complex with its cognate mRNA CGGG 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	:	3.20 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

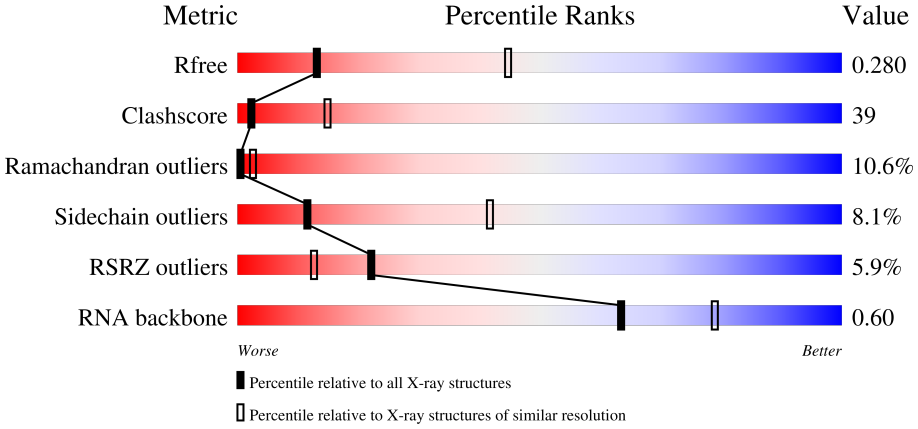
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	1523	7%, 28%, 54%, 13%, •, •
2	B	256	5%, 22%, 57%, 11%, •, 8%
3	C	239	10%, 18%, 52%, 15%, •, 13%
4	D	209	5%, 32%, 55%, 11%, •

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Mol	Chain	Length	Quality of chain
5	E	162	30% 51% 10% • 7%
6	F	101	3% 40% 51% 9%
7	G	156	4% 30% 55% 14% •
8	H	138	40% 47% 12% •
9	I	128	6% 30% 59% 10% •
10	J	105	13% 21% 56% 17% 6%
11	K	129	2% 36% 45% 11% • 8%
12	L	135	% 22% 56% 15% 7%
13	M	126	10% 27% 55% 17% •
14	N	61	5% 33% 49% 16% •
15	O	89	% 44% 49% 6% •
16	P	88	% 43% 43% 8% • 5%
17	Q	105	3% 32% 59% 6% • •
18	R	88	5% 27% 45% 10% 17%
19	S	93	10% 16% 59% 12% 13%
20	T	106	6% 29% 52% 11% • 7%
21	V	27	4% 22% 63% 7% 7%
22	X	4	50% 50%
23	Y	18	6% 11% 11% 22% 56%

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	G	3002	-	-	-	X
25	MG	G	3004	-	-	-	X
25	MG	G	3005	-	-	-	X
25	MG	G	3007	-	-	-	X
25	MG	G	3017	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	G	3018	-	-	-	X
25	MG	G	3023	-	-	-	X
25	MG	G	3030	-	-	-	X
25	MG	G	3035	-	-	-	X
25	MG	G	3036	-	-	-	X
25	MG	G	3037	-	-	-	X
25	MG	G	3040	-	-	-	X
25	MG	G	3042	-	-	-	X
25	MG	G	3047	-	-	-	X
25	MG	G	3048	-	-	-	X
25	MG	G	3049	-	-	-	X
25	MG	G	3050	-	-	-	X
25	MG	G	3054	-	-	-	X
25	MG	G	3057	-	-	-	X
25	MG	G	3061	-	-	-	X
25	MG	G	3064	-	-	-	X
25	MG	G	3067	-	-	-	X
26	K	G	3075	-	-	-	X
26	K	G	3077	-	-	-	X

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 51468 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	1484	31852	14194	5901	10285	1472	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
			Total	C	N	O	S			
7	G	155	1257	781	252	218	6	0	0	0

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

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

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
			Total	C	N	O	S			
10	J	99	793	498	157	137	1	0	0	1

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

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

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
			Total	C	N	O			
18	R	73	597	380	118	99	0	0	0

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

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

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
			Total	C	N	O			
21	V	25	209	128	51	30	0	0	1

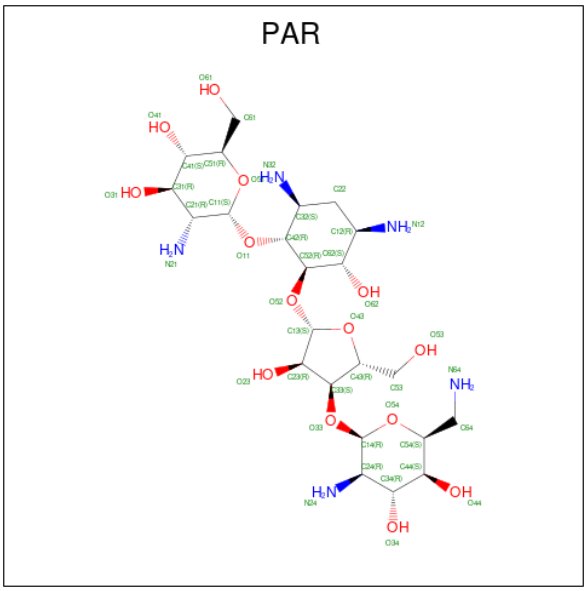
- Molecule 22 is a RNA chain called ANTICODON STEM-LOOP OF TRANSFER RNA WITH ANTICODON CCCG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	X	4	90	39	18	29	4	0	0	0

- Molecule 23 is a RNA chain called A-SITE MESSENGER RNA FRAGMENT CGGG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	Y	8	167	75	28	56	8	0	0	0

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
25	G	70	70	70	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
26	G	8	8	8	0	0

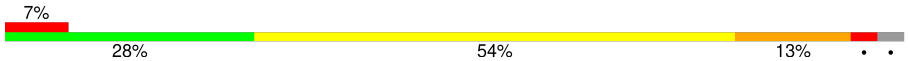
- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

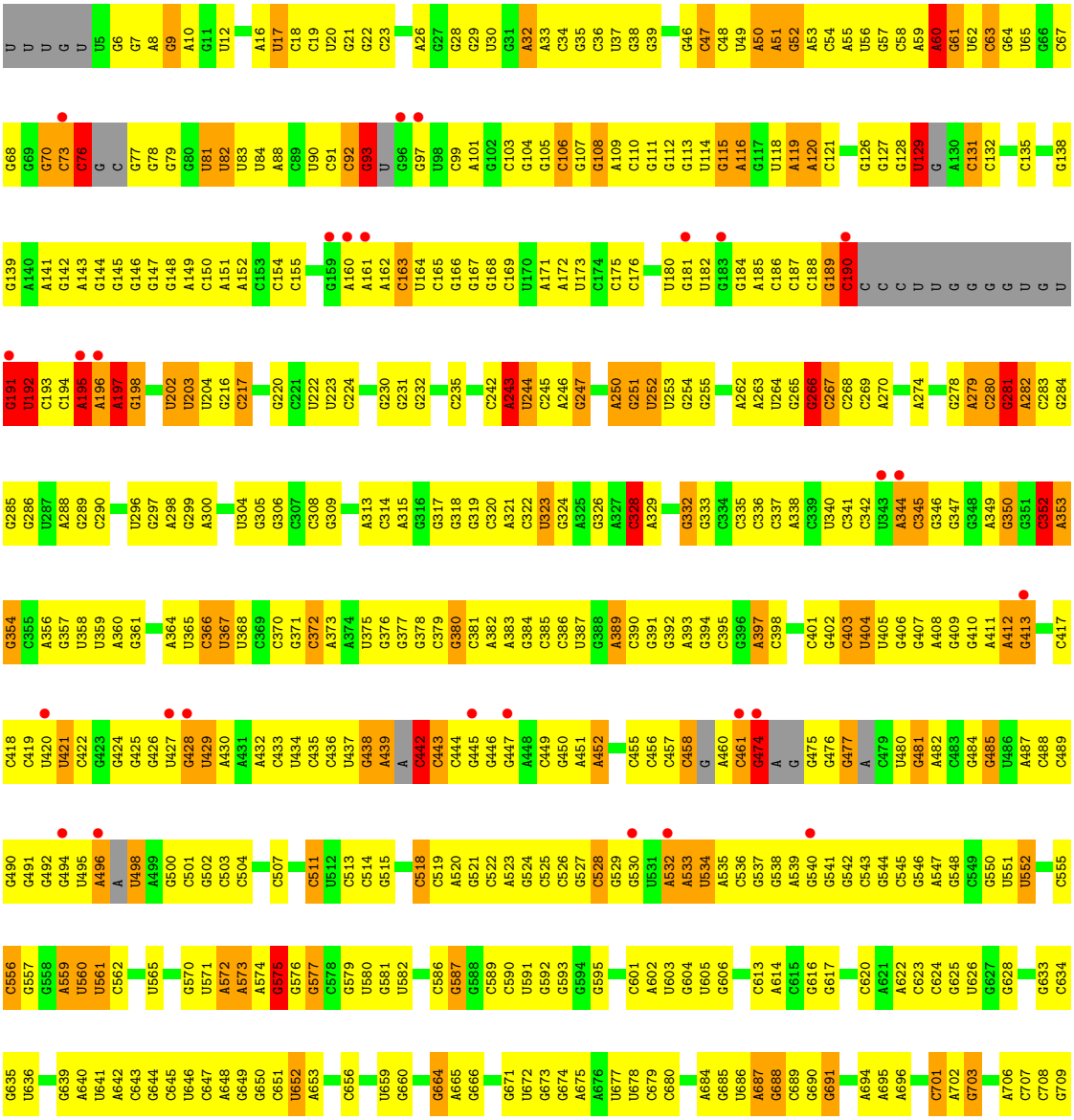
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
27	G	2	2	2	0	0

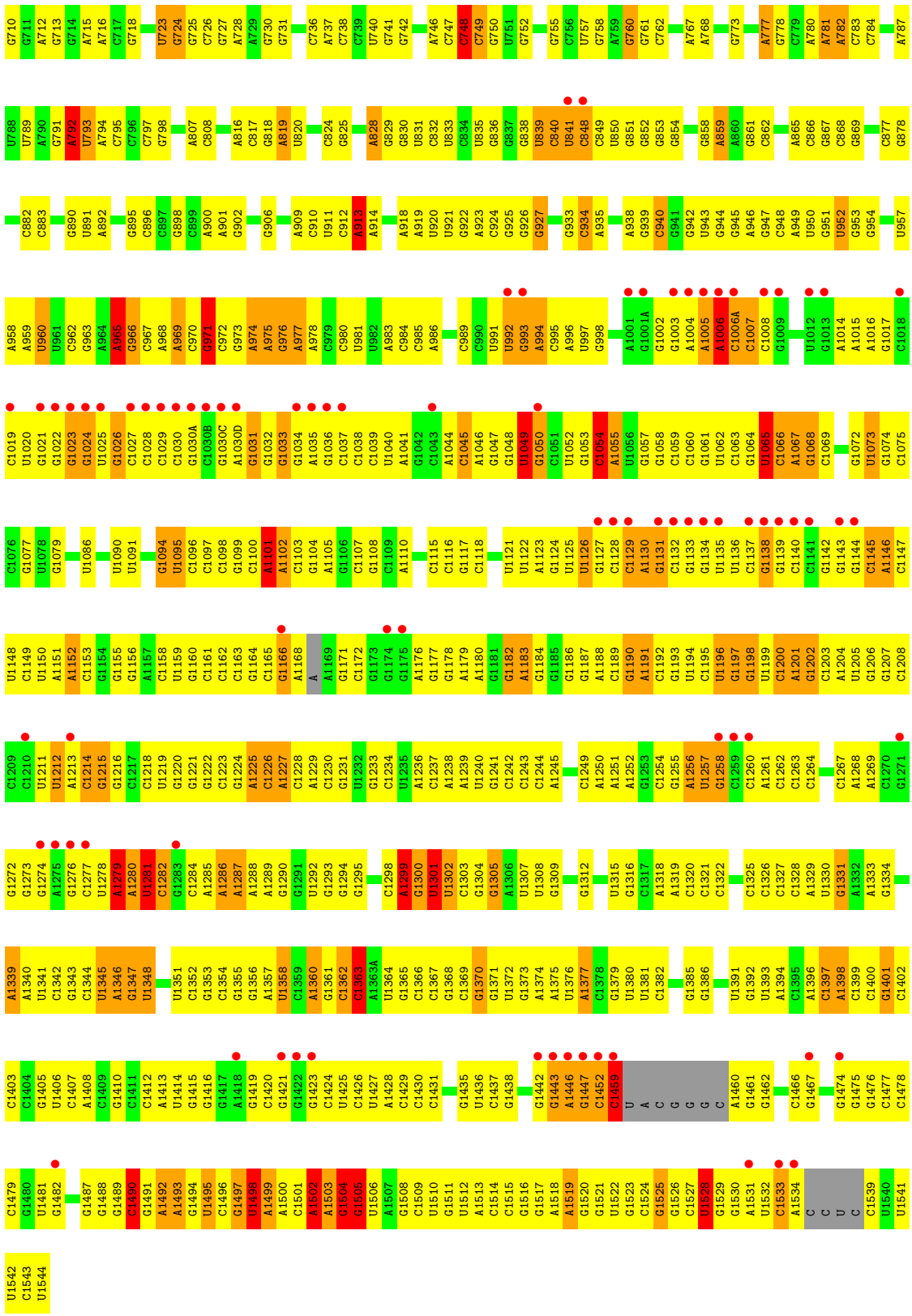
3 Residue-property plots (i)

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

- Molecule 1: 16S RIBOSOMAL RNA

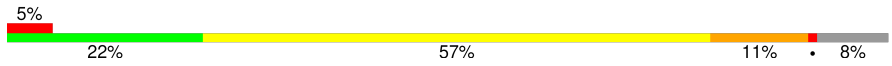
Chain A: 

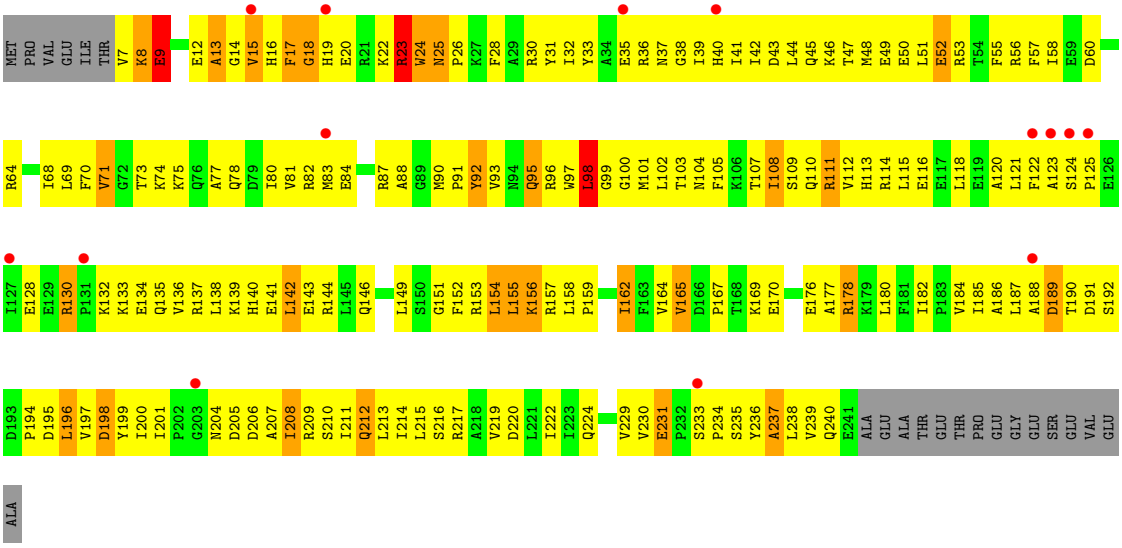




• Molecule 2: RIBOSOMAL PROTEIN S2

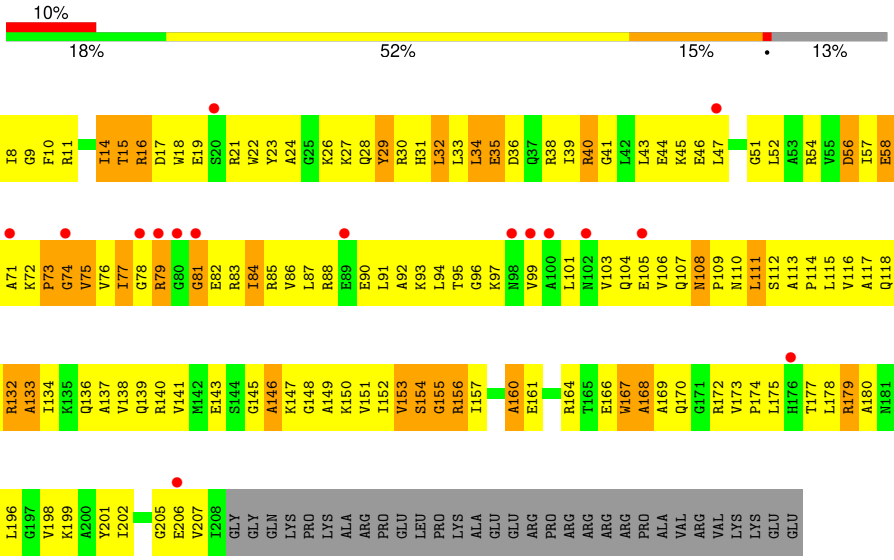
Chain B:





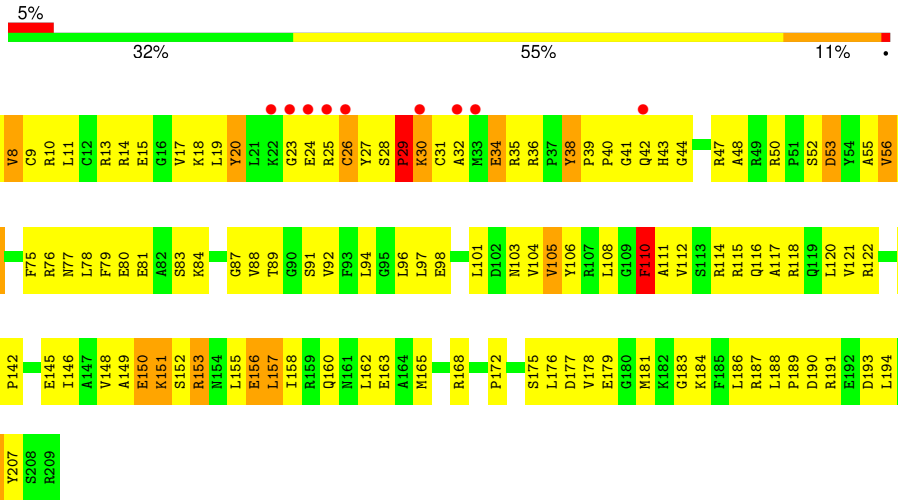
• Molecule 3: RIBOSOMAL PROTEIN S3

Chain C:



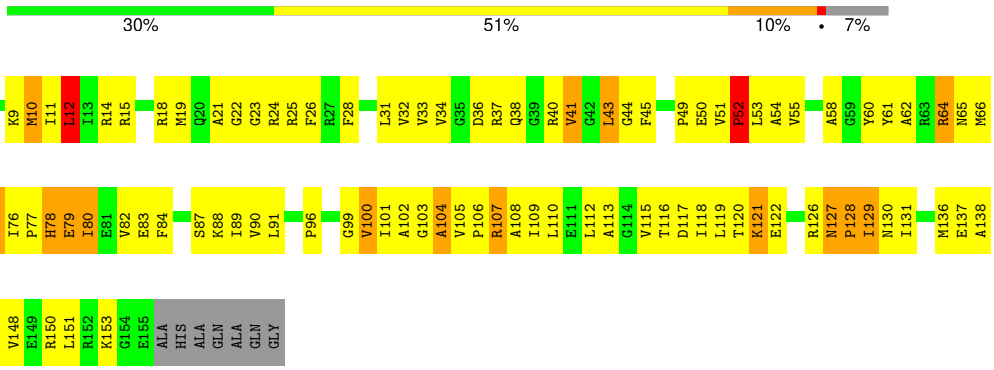
• Molecule 4: RIBOSOMAL PROTEIN S4

Chain D:



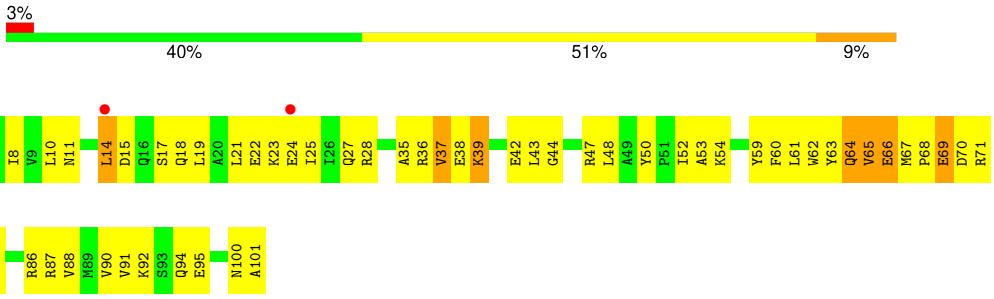
• Molecule 5: RIBOSOMAL PROTEIN S5

Chain E:



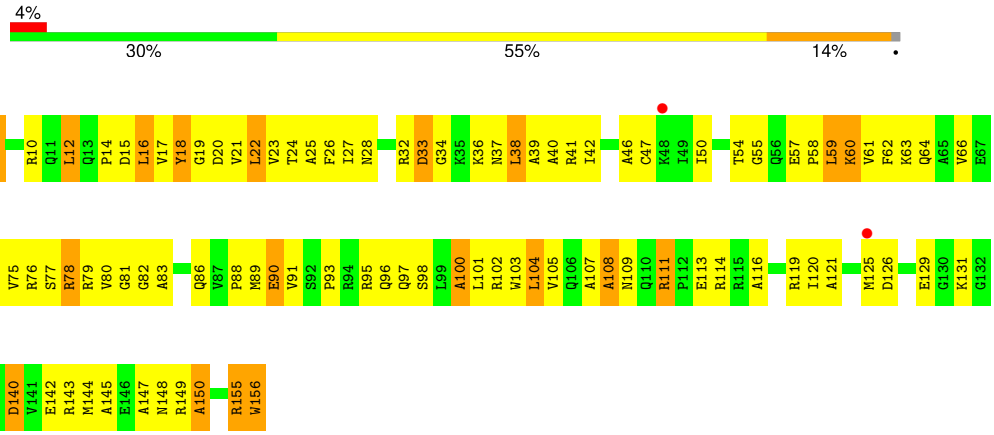
• Molecule 6: RIBOSOMAL PROTEIN S6

Chain F:



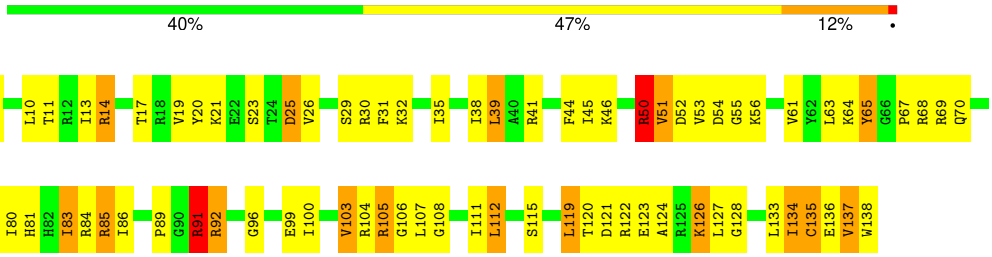
• Molecule 7: RIBOSOMAL PROTEIN S7

Chain G:



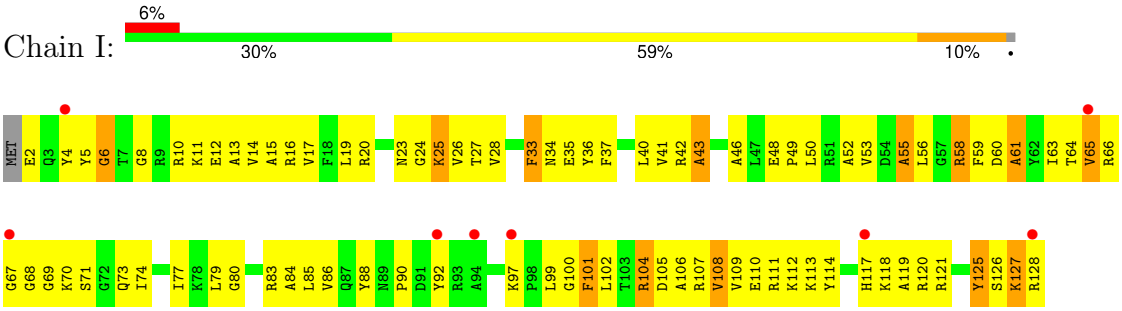
• Molecule 8: RIBOSOMAL PROTEIN S8

Chain H:



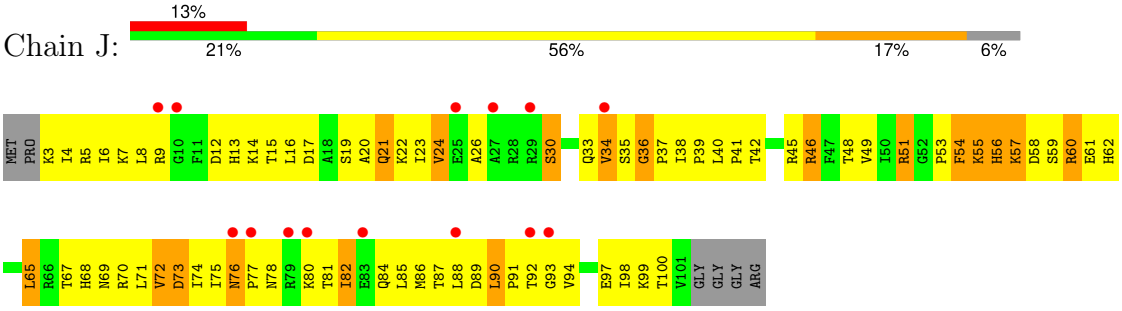
• Molecule 9: RIBOSOMAL PROTEIN S9

Chain I:



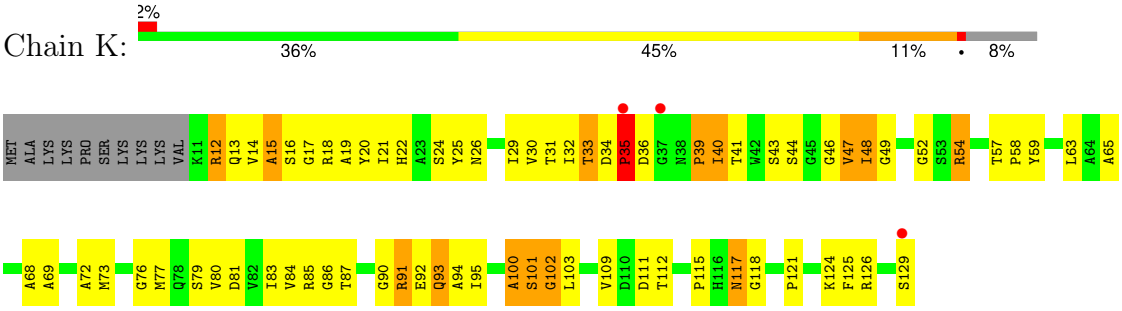
• Molecule 10: RIBOSOMAL PROTEIN S10

Chain J:



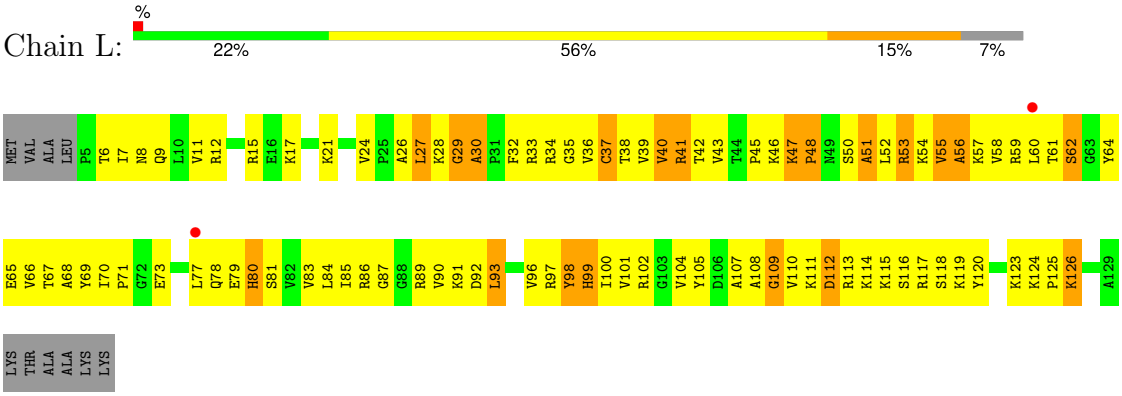
• Molecule 11: RIBOSOMAL PROTEIN S11

Chain K:



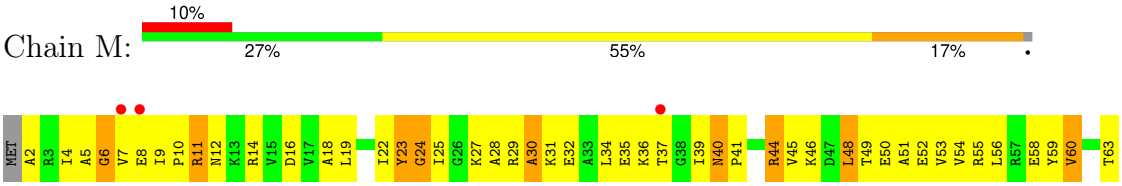
• Molecule 12: RIBOSOMAL PROTEIN S12

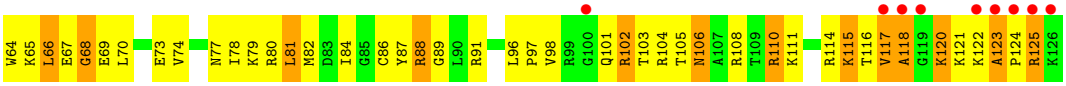
Chain L:



• Molecule 13: RIBOSOMAL PROTEIN S13

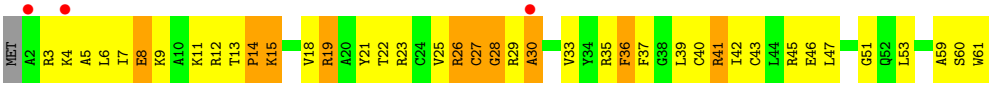
Chain M:





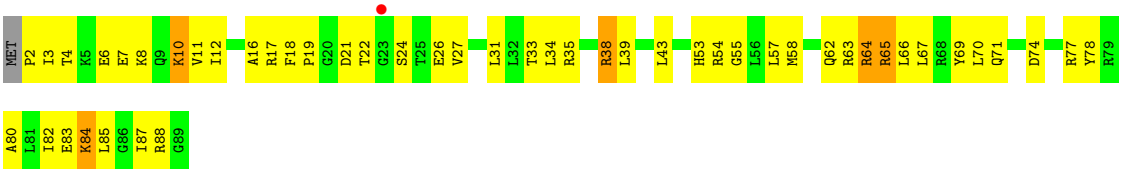
• Molecule 14: RIBOSOMAL PROTEIN S14

Chain N:



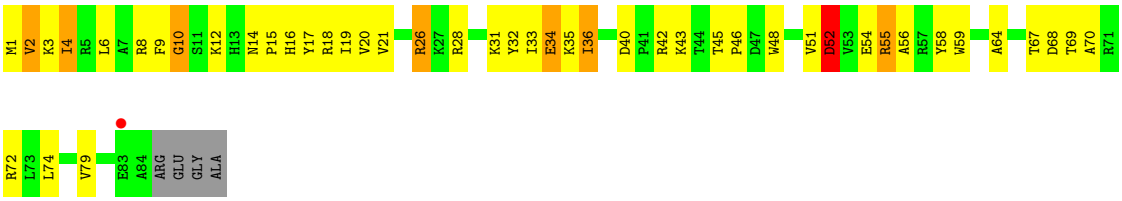
• Molecule 15: RIBOSOMAL PROTEIN S15

Chain O:



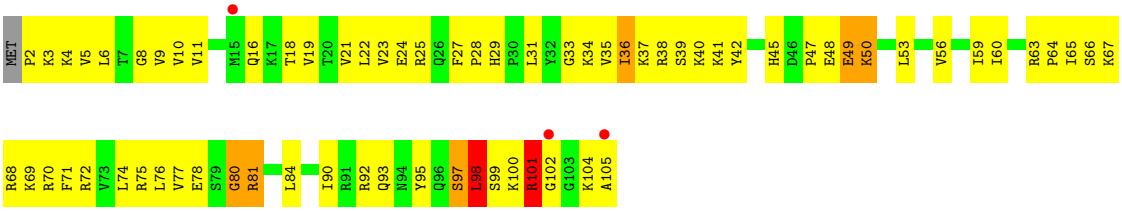
• Molecule 16: RIBOSOMAL PROTEIN S16

Chain P:



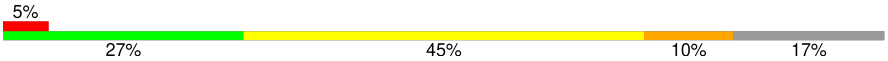
• Molecule 17: RIBOSOMAL PROTEIN S17

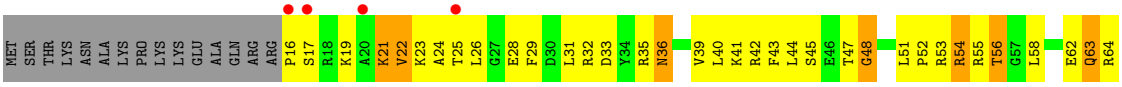
Chain Q:



• Molecule 18: RIBOSOMAL PROTEIN S18

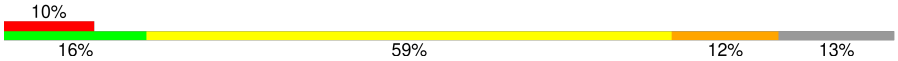
Chain R:

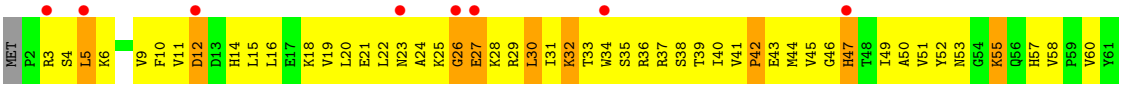


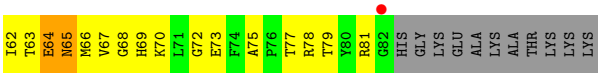


• Molecule 19: RIBOSOMAL PROTEIN S19

Chain S:

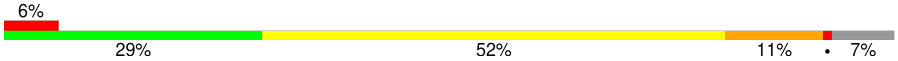


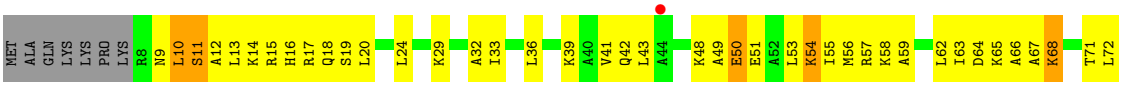


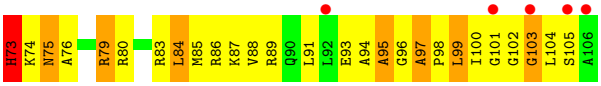


• Molecule 20: RIBOSOMAL PROTEIN S20

Chain T:

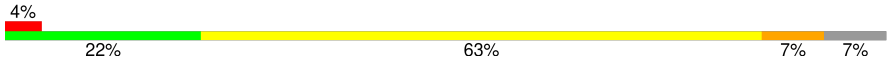






• Molecule 21: RIBOSOMAL PROTEIN THX

Chain V:



• Molecule 22: ANTICODON STEM-LOOP OF TRANSFER RNA WITH ANTICODON CCCG

Chain X:

• Molecule 23: A-SITE MESSENGER RNA FRAGMENT CGGG

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	401.90Å 401.90Å 174.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 3.20 49.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.38-3.20) 98.2 (49.38-2.80)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.282 0.238 , 0.280	Depositor DCC
R_{free} test set	17219 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	89.1	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 85.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	51468	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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 (i)

5.1 Standard geometry (i)

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

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	0.62	16/35645 (0.0%)	0.77	53/55610 (0.1%)
2	B	0.37	0/1936	0.62	0/2611
3	C	0.34	0/1637	0.58	0/2207
4	D	0.36	0/1733	0.60	0/2318
5	E	0.49	0/1163	0.75	1/1566 (0.1%)
6	F	0.32	0/856	0.58	0/1154
7	G	0.31	0/1276	0.58	0/1709
8	H	0.49	0/1136	0.76	1/1527 (0.1%)
9	I	0.33	0/1029	0.56	0/1378
10	J	0.35	0/806	0.60	0/1084
11	K	0.40	0/900	0.69	0/1213
12	L	0.42	0/987	0.71	0/1322
13	M	0.32	0/1008	0.62	0/1347
14	N	0.33	0/501	0.60	0/664
15	O	0.37	0/745	0.59	0/992
16	P	0.47	0/717	0.79	1/965 (0.1%)
17	Q	0.46	0/870	0.76	0/1159
18	R	0.35	0/603	0.63	0/799
19	S	0.32	0/662	0.58	0/892
20	T	0.41	0/764	0.70	0/1006
21	V	0.52	0/213	0.71	0/279
22	X	0.98	1/100 (1.0%)	0.93	0/153
23	Y	0.59	0/185	0.84	0/285
All	All	0.55	17/55472 (0.0%)	0.73	56/82240 (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	8	57

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	496	A	C3'-O3'	7.89	1.53	1.42
1	A	190	C	C3'-O3'	7.73	1.52	1.42
22	X	1	C	OP3-P	-7.35	1.52	1.61
1	A	129	U	C3'-O3'	7.24	1.52	1.42
1	A	73	C	C3'-O3'	7.07	1.52	1.42
1	A	191	G	O5'-C5'	6.63	1.55	1.44
1	A	191	G	O3'-P	6.46	1.69	1.61
1	A	1459	C	O5'-C5'	6.30	1.54	1.44
1	A	93	G	O5'-C5'	6.17	1.54	1.44
1	A	76	C	O5'-C5'	6.00	1.54	1.44
1	A	498	U	N1-C2	5.82	1.43	1.38
1	A	93	G	C3'-O3'	5.81	1.50	1.42
1	A	73	C	N1-C2	5.73	1.45	1.40
1	A	442	C	O5'-C5'	5.47	1.53	1.44
1	A	191	G	C5'-C4'	5.16	1.57	1.51
1	A	76	C	C5'-C4'	5.04	1.57	1.51
1	A	73	C	O3'-P	5.04	1.67	1.61

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	575	G	C2'-C3'-O3'	10.78	133.22	109.50
1	A	190	C	N1-C1'-C2'	10.38	127.49	114.00
1	A	1498	U	C2'-C3'-O3'	9.97	131.43	109.50
1	A	748	C	C2'-C3'-O3'	9.67	130.78	109.50
1	A	129	U	C2'-C3'-O3'	9.59	130.60	109.50
1	A	266	G	C2'-C3'-O3'	9.59	130.60	109.50
1	A	1528	U	C2'-C3'-O3'	9.29	129.93	109.50
1	A	115	G	C2'-C3'-O3'	9.10	129.52	109.50
1	A	281	G	C2'-C3'-O3'	8.87	129.01	109.50
1	A	366	C	C2'-C3'-O3'	8.84	128.94	109.50
1	A	1504	G	C2'-C3'-O3'	8.56	128.33	109.50
1	A	792	A	C2'-C3'-O3'	8.49	128.18	109.50
1	A	197	A	C2'-C3'-O3'	8.10	127.32	109.50
1	A	243	A	C2'-C3'-O3'	8.01	127.11	109.50
1	A	108	G	O4'-C1'-N9	7.70	114.36	108.20
1	A	60	A	C2'-C3'-O3'	7.25	125.44	109.50
1	A	965	A	C2'-C3'-O3'	7.21	125.37	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1101	A	C2'-C3'-O3'	7.20	125.33	109.50
1	A	1006	A	N9-C1'-C2'	6.93	123.01	114.00
1	A	192	U	O5'-P-OP1	-6.70	99.67	105.70
1	A	1505	G	C2'-C3'-O3'	6.42	123.96	113.70
1	A	389	A	C5'-C4'-C3'	6.20	125.91	116.00
1	A	971	G	N9-C1'-C2'	6.15	122.00	114.00
1	A	76	C	C5'-C4'-C3'	6.03	125.65	116.00
1	A	1502	A	N9-C1'-C2'	6.01	121.81	114.00
1	A	1299	A	N9-C1'-C2'	5.98	121.78	114.00
1	A	1054	C	C2'-C3'-O3'	5.93	123.19	113.70
1	A	129	U	C4'-C3'-O3'	5.90	124.81	113.00
1	A	281	G	C4'-C3'-O3'	5.88	124.76	113.00
1	A	1490	C	C5'-C4'-O4'	-5.85	102.08	109.10
1	A	73	C	C2'-C3'-O3'	5.84	123.05	113.70
1	A	191	G	C4'-C3'-O3'	5.79	124.57	113.00
1	A	1363	C	O4'-C1'-N1	5.76	112.81	108.20
1	A	913	A	C2'-C3'-O3'	5.65	122.73	113.70
1	A	51	A	N9-C1'-C2'	5.64	121.34	114.00
1	A	1504	G	C4'-C3'-O3'	5.62	124.23	113.00
1	A	108	G	O4'-C4'-C3'	-5.61	98.39	104.00
1	A	1279	A	N9-C1'-C2'	5.61	121.29	114.00
1	A	1459	C	C5'-C4'-O4'	-5.55	102.44	109.10
1	A	575	G	O4'-C1'-N9	-5.50	103.80	108.20
1	A	498	U	O4'-C1'-N1	5.49	112.59	108.20
8	H	134	ILE	N-CA-C	5.44	125.69	111.00
1	A	1363	C	C5'-C4'-O4'	5.44	115.63	109.10
1	A	1301	U	C2'-C3'-O3'	5.42	122.37	113.70
1	A	328	C	N1-C1'-C2'	5.37	120.98	114.00
1	A	1065	U	C1'-O4'-C4'	-5.37	105.60	109.90
1	A	1166	G	N9-C1'-C2'	-5.35	106.11	112.00
5	E	12	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	572	A	N9-C1'-C2'	5.25	120.83	114.00
1	A	694	A	C5'-C4'-C3'	-5.24	107.61	116.00
16	P	4	ILE	N-CA-C	-5.16	97.08	111.00
1	A	820	U	N1-C1'-C2'	5.09	120.62	114.00
1	A	1049	U	N1-C1'-C2'	5.09	120.61	114.00
1	A	1505	G	O5'-P-OP2	5.06	116.77	110.70
1	A	1442	G	N9-C1'-C2'	5.04	120.55	114.00
1	A	474	G	O4'-C1'-N9	-5.03	104.18	108.20

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	115	G	C3'
1	A	129	U	C3'
1	A	281	G	C3'
1	A	748	C	C3'
1	A	1006	A	C1'
1	A	1498	U	C3'
1	A	1504	G	C3'
1	A	1528	U	C3'

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	C	Sidechain
1	A	1073	U	Sidechain
1	A	1077	G	Sidechain
1	A	128	G	Sidechain
1	A	1281	U	Sidechain
1	A	129	U	Sidechain
1	A	1299	A	Sidechain
1	A	1300	G	Sidechain
1	A	1339	A	Sidechain
1	A	1345	U	Sidechain
1	A	1358	U	Sidechain
1	A	1377	A	Sidechain
1	A	1394	A	Sidechain
1	A	1495	U	Sidechain
1	A	1502	A	Sidechain
1	A	1519	A	Sidechain
1	A	1525	G	Sidechain
1	A	17	U	Sidechain
1	A	190	C	Sidechain
1	A	191	G	Sidechain
1	A	195	A	Sidechain
1	A	197	A	Sidechain
1	A	281	G	Sidechain
1	A	290	C	Sidechain
1	A	323	U	Sidechain
1	A	352	C	Sidechain
1	A	380	G	Sidechain
1	A	403	C	Sidechain
1	A	404	U	Sidechain
1	A	474	G	Sidechain
1	A	481	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	507	C	Sidechain
1	A	528	C	Sidechain
1	A	552	U	Sidechain
1	A	556	C	Sidechain
1	A	561	U	Sidechain
1	A	565	U	Sidechain
1	A	573	A	Sidechain
1	A	575	G	Sidechain
1	A	582	U	Sidechain
1	A	587	G	Sidechain
1	A	595	G	Sidechain
1	A	652	U	Sidechain
1	A	664	G	Sidechain
1	A	691	G	Sidechain
1	A	70	G	Sidechain
1	A	724	G	Sidechain
1	A	727	G	Sidechain
1	A	760	G	Sidechain
1	A	773	G	Sidechain
1	A	777	A	Sidechain
1	A	831	U	Sidechain
1	A	835	U	Sidechain
1	A	898	G	Sidechain
1	A	93	G	Sidechain
1	A	940	C	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	31852	0	16122	1389	0
2	B	1901	0	1951	247	0
3	C	1613	0	1677	261	0
4	D	1703	0	1764	178	0
5	E	1147	0	1207	112	0
6	F	843	0	857	75	0
7	G	1257	0	1296	141	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1116	0	1177	114	0
9	I	1011	0	1043	134	0
10	J	793	0	835	145	0
11	K	885	0	904	87	0
12	L	971	0	1057	154	0
13	M	997	0	1072	115	0
14	N	492	0	531	66	0
15	O	734	0	771	65	0
16	P	701	0	720	58	0
17	Q	857	0	930	83	0
18	R	597	0	666	60	0
19	S	648	0	673	93	0
20	T	762	0	859	84	0
21	V	209	0	221	19	0
22	X	90	0	45	11	0
23	Y	167	0	87	14	0
24	A	42	0	45	0	0
25	G	70	0	0	0	0
26	G	8	0	0	0	0
27	G	2	0	0	0	0
All	All	51468	0	36510	3377	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 39.

All (3377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:G:H2'	1:A:190:C:C6	1.68	1.27
3:C:27:LYS:HA	3:C:30:ARG:HH12	1.09	1.13
10:J:38:ILE:HD11	10:J:71:LEU:HB2	1.20	1.11
1:A:1305:G:H22	1:A:1331:G:H2'	1.02	1.10
1:A:1356:G:H2'	1:A:1357:A:C8	1.88	1.08
1:A:189:G:H2'	1:A:190:C:H6	0.91	1.07
12:L:41:ARG:HG2	12:L:42:THR:H	1.20	1.06
1:A:1277:C:H2'	1:A:1278:U:H5'	1.38	1.06
1:A:1305:G:N2	1:A:1331:G:H2'	1.71	1.05
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.38	1.05
7:G:111:ARG:HB3	7:G:111:ARG:HH11	1.22	1.03
1:A:189:G:C2	1:A:190:C:H1'	1.94	1.02
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:48:ILE:HG22	11:K:49:GLY:H	1.20	1.02
1:A:530:G:O6	22:X:3:G:H1'	1.60	1.02
1:A:1064:G:H4'	1:A:1065:U:H5'	1.43	1.01
2:B:80:ILE:HG23	2:B:212:GLN:HE21	1.22	1.00
1:A:191:G:O4'	20:T:105:SER:HA	1.60	1.00
6:F:6:VAL:HG13	6:F:90:VAL:HG22	1.44	1.00
1:A:972:C:H4'	10:J:57:LYS:HG2	1.44	0.98
1:A:522:C:H41	12:L:53:ARG:HH22	1.09	0.98
1:A:1216:G:H5"	14:N:5:ALA:HB2	1.45	0.98
1:A:1490:C:H6	1:A:1490:C:H5'	1.26	0.98
11:K:20:TYR:HE2	11:K:83:ILE:HD12	1.27	0.98
12:L:60:LEU:HD21	12:L:66:VAL:HG22	1.44	0.97
1:A:455:C:H42	1:A:477:G:H1	1.10	0.97
4:D:62:GLN:HA	4:D:62:GLN:HE21	1.28	0.97
14:N:3:ARG:H	14:N:3:ARG:HD2	1.26	0.97
3:C:78:GLY:HA3	3:C:82:GLU:HB3	1.47	0.97
5:E:80:ILE:HD12	5:E:138:ALA:HB1	1.47	0.97
2:B:68:ILE:H	2:B:90:MET:HE1	1.27	0.96
1:A:129:U:H5'	17:Q:3:LYS:NZ	1.79	0.96
1:A:266:G:C8	1:A:266:G:H5"	2.01	0.96
12:L:93:LEU:HD23	12:L:93:LEU:H	1.29	0.96
14:N:26:ARG:HH11	14:N:47:LEU:HD21	1.28	0.96
2:B:82:ARG:HA	2:B:92:TYR:HE1	1.30	0.95
19:S:15:LEU:HA	19:S:18:LYS:HB3	1.45	0.95
7:G:75:VAL:HG11	7:G:86:GLN:HB3	1.48	0.95
1:A:1030:C:H2'	1:A:1030(A):G:C8	2.02	0.95
2:B:18:GLY:HA2	2:B:41:ILE:HA	1.48	0.95
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.46	0.95
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.48	0.95
2:B:178:ARG:HH11	2:B:178:ARG:HG3	1.30	0.94
13:M:52:GLU:HG2	13:M:55:ARG:HH21	1.32	0.94
7:G:14:PRO:HA	7:G:21:VAL:HG12	1.48	0.94
10:J:4:ILE:HD12	10:J:74:ILE:HB	1.50	0.94
1:A:112:G:H21	1:A:354:G:H5'	1.32	0.94
1:A:918:A:H2'	1:A:919:A:C8	2.03	0.93
11:K:87:THR:HG23	11:K:91:ARG:HH21	1.33	0.93
2:B:154:LEU:HD23	2:B:154:LEU:H	1.32	0.93
1:A:1369:C:H2'	1:A:1370:G:C8	2.04	0.93
1:A:991:U:N3	1:A:1212:U:H1'	1.81	0.93
8:H:69:ARG:NH1	8:H:69:ARG:HB2	1.83	0.93
19:S:33:THR:HG22	19:S:35:SER:H	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1277:C:C2'	1:A:1278:U:H5'	1.97	0.93
3:C:84:ILE:HG12	3:C:88:ARG:HD2	1.48	0.93
1:A:991:U:H3	1:A:1212:U:H1'	1.33	0.92
13:M:117:VAL:HG23	13:M:118:ALA:H	1.33	0.92
1:A:1006:A:H5'	1:A:1006(A):C:C5'	2.00	0.92
1:A:92:C:H2'	1:A:93:G:N7	1.85	0.92
8:H:69:ARG:HB2	8:H:69:ARG:HH11	1.35	0.91
16:P:51:VAL:O	16:P:52:ASP:HB3	1.69	0.90
11:K:14:VAL:HG21	11:K:40:ILE:HD11	1.53	0.90
1:A:1148:U:H2'	1:A:1149:C:O4'	1.72	0.90
1:A:939:G:H5"	7:G:102:ARG:HH22	1.36	0.90
1:A:1502:A:H2	1:A:1505:G:H1	1.16	0.89
10:J:90:LEU:H	10:J:91:PRO:HD2	1.38	0.89
2:B:102:LEU:HD21	2:B:162:ILE:HD11	1.53	0.89
5:E:129:ILE:H	5:E:129:ILE:HD12	1.37	0.89
1:A:188:C:H2'	1:A:189:G:O2'	1.73	0.88
1:A:1356:G:H2'	1:A:1357:A:H8	1.36	0.88
2:B:69:LEU:HD23	2:B:70:PHE:N	1.89	0.88
3:C:27:LYS:HA	3:C:30:ARG:NH1	1.88	0.88
11:K:121:PRO:HG2	11:K:126:ARG:HG3	1.53	0.88
1:A:524:G:H2'	1:A:525:C:C6	2.09	0.88
1:A:1366:C:H2'	1:A:1367:C:H6	1.38	0.88
1:A:1368:G:OP2	9:I:112:LYS:HD3	1.74	0.88
22:X:2:G:H1	23:Y:36:C:H42	1.20	0.88
1:A:877:C:O2	8:H:3:THR:HG21	1.73	0.88
8:H:46:LYS:HG3	8:H:64:LYS:HB3	1.55	0.88
18:R:87:ARG:HB3	18:R:87:ARG:HH11	1.38	0.88
1:A:1129:C:H1'	1:A:1132:C:H5	1.39	0.88
1:A:707:C:H4'	11:K:20:TYR:CD1	2.09	0.87
12:L:47:LYS:HB2	12:L:48:PRO:HD3	1.56	0.87
1:A:523:A:H61	12:L:92:ASP:HB2	1.38	0.87
1:A:501:C:H2'	1:A:502:G:H8	1.38	0.87
1:A:412:A:C2	4:D:35:ARG:HG3	2.10	0.86
2:B:197:VAL:HB	2:B:200:ILE:HD11	1.56	0.86
1:A:191:G:H21	20:T:85:MET:HE3	1.37	0.86
7:G:90:GLU:H	7:G:155:ARG:HH22	1.19	0.86
1:A:1459:C:H2'	1:A:1460:A:H8	1.40	0.86
15:O:65:ARG:HH11	15:O:65:ARG:HB2	1.38	0.86
1:A:1489:G:H2'	1:A:1490:C:H5"	1.57	0.86
13:M:81:LEU:HD23	13:M:81:LEU:H	1.39	0.86
1:A:954:G:H21	1:A:1227:A:H62	1.20	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:117:HIS:HB2	9:I:121:ARG:HG2	1.56	0.86
1:A:1006:A:H5'	1:A:1006(A):C:H5"	1.56	0.86
3:C:153:VAL:HG12	3:C:154:SER:H	1.39	0.86
1:A:1147:C:HO2'	9:I:5:TYR:HH	1.20	0.85
9:I:79:LEU:HD11	9:I:83:ARG:HD2	1.58	0.85
11:K:20:TYR:CE2	11:K:83:ILE:HD12	2.10	0.85
20:T:51:GLU:HA	20:T:54:LYS:HB2	1.57	0.85
1:A:1489:G:C2'	1:A:1490:C:H5"	2.06	0.85
3:C:191:THR:HG22	3:C:192:THR:N	1.90	0.85
1:A:532:A:H62	3:C:161:GLU:HB2	1.41	0.85
1:A:266:G:H5"	1:A:266:G:H8	1.40	0.85
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.57	0.85
14:N:37:PHE:HE2	14:N:53:LEU:HD13	1.42	0.85
3:C:191:THR:HG22	3:C:192:THR:H	1.41	0.85
1:A:1391:U:H2'	1:A:1392:G:C8	2.12	0.85
15:O:26:GLU:OE1	15:O:77:ARG:HD2	1.77	0.84
1:A:1226:C:H4'	1:A:1227:A:OP1	1.77	0.84
6:F:18:GLN:HA	6:F:21:LEU:HB3	1.59	0.84
10:J:7:LYS:HB2	10:J:97:GLU:HB2	1.59	0.84
3:C:91:LEU:HD23	3:C:92:ALA:H	1.39	0.84
12:L:6:THR:OG1	12:L:9:GLN:HG3	1.77	0.84
1:A:1064:G:H4'	1:A:1065:U:C5'	2.07	0.84
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.59	0.84
12:L:93:LEU:HD23	12:L:93:LEU:N	1.92	0.84
18:R:87:ARG:HB3	18:R:87:ARG:NH1	1.93	0.84
3:C:6:HIS:HD2	3:C:9:GLY:H	1.26	0.84
3:C:179:ARG:HH11	3:C:206:GLU:HG2	1.41	0.84
10:J:62:HIS:HB3	14:N:59:ALA:HB3	1.60	0.84
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.57	0.84
1:A:189:G:C2'	1:A:190:C:H6	1.84	0.83
1:A:474:G:N3	1:A:474:G:H5"	1.93	0.83
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.61	0.83
14:N:27:CYS:SG	14:N:29:ARG:HG3	2.18	0.83
2:B:77:ALA:HB1	2:B:80:ILE:HD12	1.61	0.83
14:N:27:CYS:SG	14:N:28:GLY:N	2.52	0.83
1:A:1443:G:H4'	1:A:1446:A:H5'	1.61	0.83
1:A:1459:C:H2'	1:A:1460:A:C8	2.13	0.83
4:D:162:LEU:HD13	4:D:181:MET:HG2	1.61	0.82
10:J:38:ILE:CD1	10:J:71:LEU:HB2	2.07	0.82
1:A:1250:A:H2'	1:A:1251:A:C8	2.15	0.82
21:V:6:ARG:HH21	21:V:7:ARG:HB3	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:GLU:HB2	3:C:65:ALA:HB3	1.59	0.82
10:J:7:LYS:HA	10:J:71:LEU:HD23	1.60	0.82
17:Q:63:ARG:O	17:Q:65:ILE:HD12	1.79	0.82
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.61	0.82
3:C:3:ASN:HD22	3:C:3:ASN:N	1.78	0.82
2:B:82:ARG:HA	2:B:92:TYR:CE1	2.15	0.81
8:H:69:ARG:HH11	8:H:69:ARG:CB	1.92	0.81
10:J:8:LEU:HD12	10:J:70:ARG:HB2	1.61	0.81
11:K:18:ARG:HG3	11:K:33:THR:HG23	1.62	0.81
19:S:64:GLU:O	19:S:67:VAL:HG23	1.80	0.81
1:A:532:A:H62	3:C:161:GLU:CB	1.93	0.81
4:D:110:PHE:HD1	4:D:110:PHE:H	1.26	0.81
10:J:5:ARG:H	10:J:100:THR:HA	1.46	0.81
12:L:45:PRO:HG2	12:L:51:ALA:N	1.96	0.81
1:A:1435:G:H2'	1:A:1436:U:C6	2.16	0.81
4:D:18:LYS:HD3	4:D:20:TYR:HE2	1.46	0.81
13:M:2:ALA:O	13:M:10:PRO:HD2	1.80	0.81
1:A:189:G:C2'	1:A:190:C:C6	2.60	0.81
1:A:1003:G:H2'	1:A:1004:A:H5"	1.62	0.81
1:A:447:G:H2'	1:A:485:G:N2	1.96	0.81
7:G:90:GLU:N	7:G:155:ARG:HH22	1.78	0.81
1:A:76:C:H42	1:A:93:G:H1	1.27	0.80
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.63	0.80
9:I:127:LYS:H	9:I:127:LYS:HD2	1.46	0.80
1:A:579:G:H5'	1:A:728:A:H1'	1.64	0.80
11:K:14:VAL:HG21	11:K:40:ILE:CD1	2.11	0.80
1:A:673:G:H2'	1:A:674:G:C8	2.16	0.80
1:A:957:U:H3	1:A:960:U:H5"	1.45	0.80
9:I:48:GLU:N	9:I:49:PRO:HD2	1.97	0.80
3:C:130:VAL:HG11	3:C:157:ILE:HG23	1.64	0.80
20:T:39:LYS:HE2	20:T:55:ILE:HD13	1.64	0.80
2:B:151:GLY:C	2:B:153:ARG:H	1.84	0.80
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.63	0.80
8:H:50:ARG:O	8:H:51:VAL:HG23	1.82	0.79
1:A:265:G:H2'	1:A:267:C:H5	1.45	0.79
1:A:1498:U:H4'	1:A:1519:A:H2	1.45	0.79
12:L:8:ASN:O	12:L:12:ARG:HG3	1.81	0.79
1:A:437:U:H3	1:A:496:A:N6	1.80	0.79
1:A:129:U:H5'	17:Q:3:LYS:HZ1	1.44	0.79
1:A:191:G:N2	20:T:85:MET:CE	2.45	0.79
10:J:3:LYS:HD3	10:J:76:ASN:H	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:90:LEU:H	10:J:91:PRO:CD	1.94	0.79
1:A:420:U:H4'	1:A:421:U:H5	1.46	0.79
1:A:1006:A:C5'	1:A:1006(A):C:H5"	2.12	0.79
1:A:1129:C:O5'	1:A:1130:A:H5'	1.83	0.79
1:A:1191:A:H2'	1:A:1192:C:H6	1.47	0.79
7:G:16:LEU:H	7:G:16:LEU:HD22	1.47	0.79
13:M:14:ARG:H	13:M:44:ARG:HH21	1.30	0.79
1:A:1057:G:O2'	1:A:1058:G:H5'	1.83	0.79
1:A:9:G:H5"	5:E:122:GLU:OE2	1.83	0.78
3:C:57:ILE:HG23	3:C:64:VAL:HG13	1.63	0.78
1:A:81:U:H2'	1:A:83:U:OP2	1.82	0.78
1:A:1006:A:H4'	1:A:1006:A:OP1	1.83	0.78
1:A:1492:A:N3	22:X:2:G:O2'	2.15	0.78
1:A:1532:U:O2'	1:A:1533:C:H4'	1.83	0.78
13:M:14:ARG:N	13:M:44:ARG:HH21	1.81	0.78
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.64	0.78
1:A:1065:U:H4'	1:A:1066:C:O5'	1.82	0.78
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.64	0.78
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.65	0.78
3:C:117:ALA:HB1	3:C:187:ALA:HB2	1.66	0.78
14:N:3:ARG:H	14:N:3:ARG:CD	1.94	0.78
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.66	0.78
1:A:781:A:H2'	1:A:782:A:H5'	1.65	0.78
1:A:489:C:H2'	1:A:490:G:H8	1.49	0.78
2:B:213:LEU:HD23	2:B:214:ILE:N	1.98	0.78
1:A:383:A:H2'	1:A:384:G:H5'	1.66	0.78
1:A:407:G:O2'	4:D:116:GLN:HG3	1.84	0.78
1:A:939:G:H5"	7:G:102:ARG:NH2	1.98	0.78
9:I:102:LEU:HD23	9:I:102:LEU:H	1.49	0.78
7:G:101:LEU:HA	7:G:104:LEU:HD12	1.66	0.77
9:I:15:ALA:HA	9:I:65:VAL:HA	1.66	0.77
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.48	0.77
1:A:190:C:H6	1:A:190:C:O5'	1.68	0.77
15:O:10:LYS:HE3	15:O:11:VAL:HG22	1.66	0.77
17:Q:76:LEU:HD23	17:Q:77:VAL:N	2.00	0.77
13:M:50:GLU:O	13:M:54:VAL:HG23	1.84	0.77
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.67	0.77
4:D:131:ARG:HD2	4:D:131:ARG:N	2.00	0.77
1:A:474:G:H5'	1:A:475:G:N7	1.99	0.77
1:A:1459:C:C6	1:A:1459:C:O5'	2.38	0.77
4:D:62:GLN:HA	4:D:62:GLN:NE2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:11:ARG:NH1	13:M:11:ARG:HA	2.00	0.77
1:A:995:C:H1'	14:N:4:LYS:HE2	1.66	0.77
1:A:1225:A:H2'	1:A:1225:A:N3	1.99	0.77
1:A:1278:U:H5"	1:A:1279:A:O4'	1.85	0.77
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.49	0.77
10:J:16:LEU:HD21	10:J:94:VAL:HG11	1.64	0.77
1:A:91:C:H2'	1:A:92:C:C6	2.19	0.77
1:A:149:A:H2'	1:A:150:C:C6	2.21	0.76
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.65	0.76
1:A:580:U:H2'	1:A:581:G:O4'	1.85	0.76
1:A:1128:C:O2'	1:A:1129:C:H5"	1.85	0.76
14:N:3:ARG:HD2	14:N:3:ARG:N	1.98	0.76
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.00	0.76
7:G:89:MET:HA	7:G:155:ARG:CZ	2.15	0.76
1:A:1347:G:N2	1:A:1373:G:H2'	2.00	0.76
3:C:179:ARG:HD3	3:C:207:VAL:H	1.50	0.76
7:G:116:ALA:HA	7:G:119:ARG:HH21	1.50	0.76
9:I:71:SER:HA	9:I:74:ILE:HD12	1.67	0.76
1:A:1004:A:H1'	1:A:1036:G:H1	1.50	0.76
3:C:7:PRO:HG2	3:C:184:TYR:HB2	1.66	0.76
12:L:83:VAL:HG22	12:L:84:LEU:H	1.50	0.76
17:Q:81:ARG:HG3	17:Q:81:ARG:O	1.86	0.76
3:C:26:LYS:HE2	3:C:26:LYS:H	1.48	0.76
3:C:27:LYS:CA	3:C:30:ARG:HH12	1.94	0.76
12:L:46:LYS:HG2	12:L:47:LYS:N	2.01	0.76
12:L:60:LEU:CD2	12:L:66:VAL:HG22	2.16	0.75
1:A:555:C:H2'	1:A:556:C:C6	2.21	0.75
13:M:59:TYR:O	13:M:63:THR:HG22	1.85	0.75
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.20	0.75
2:B:92:TYR:CD2	2:B:151:GLY:HA3	2.20	0.75
3:C:191:THR:CG2	3:C:192:THR:H	1.98	0.75
8:H:29:SER:HB3	8:H:32:LYS:HG3	1.68	0.75
1:A:1211:U:H1'	1:A:1213:A:C2	2.21	0.75
4:D:39:PRO:HG2	4:D:44:GLY:HA2	1.67	0.75
1:A:191:G:N2	20:T:85:MET:HE3	2.01	0.75
5:E:9:LYS:HD3	5:E:112:LEU:HD21	1.68	0.75
12:L:36:VAL:O	12:L:37:CYS:HB2	1.87	0.75
20:T:14:LYS:O	20:T:18:GLN:HG3	1.86	0.75
1:A:129:U:H5'	17:Q:3:LYS:HZ3	1.50	0.75
1:A:794:A:H2'	1:A:795:C:C6	2.22	0.75
1:A:838:G:H2'	1:A:839:U:H5"	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:48:ILE:HG22	11:K:49:GLY:N	1.97	0.75
1:A:1391:U:H2'	1:A:1392:G:H8	1.49	0.74
1:A:1425:U:H3	1:A:1475:G:H1	1.34	0.74
1:A:420:U:H4'	1:A:421:U:C5	2.22	0.74
20:T:73:HIS:O	20:T:74:LYS:HG2	1.86	0.74
1:A:404:U:O2'	1:A:405:U:H5'	1.88	0.74
2:B:19:HIS:HD2	2:B:189:ASP:HB2	1.51	0.74
8:H:127:LEU:H	8:H:127:LEU:HD22	1.50	0.74
11:K:43:SER:HA	11:K:47:VAL:HG21	1.68	0.74
11:K:54:ARG:HB3	11:K:54:ARG:HH11	1.52	0.74
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.53	0.74
2:B:188:ALA:HB1	2:B:192:SER:OG	1.86	0.74
12:L:41:ARG:HG2	12:L:42:THR:N	2.00	0.74
14:N:37:PHE:CE2	14:N:53:LEU:HD13	2.22	0.74
17:Q:66:SER:HB3	17:Q:69:LYS:HB3	1.68	0.74
3:C:6:HIS:CD2	3:C:9:GLY:H	2.05	0.74
7:G:111:ARG:HB3	7:G:111:ARG:NH1	2.01	0.74
1:A:35:G:N3	12:L:118:SER:HB2	2.02	0.74
1:A:1030(A):G:N2	1:A:1030(C):G:H3'	2.02	0.74
2:B:95:GLN:O	2:B:96:ARG:HD2	1.88	0.74
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.22	0.74
2:B:156:LYS:O	2:B:156:LYS:HD3	1.88	0.74
7:G:24:THR:HA	7:G:27:ILE:HD12	1.69	0.74
10:J:90:LEU:N	10:J:91:PRO:HD2	2.03	0.74
1:A:175:C:H2'	1:A:176:C:H6	1.52	0.74
2:B:18:GLY:HA2	2:B:40:HIS:O	1.88	0.74
5:E:41:VAL:HG13	5:E:113:ALA:HA	1.70	0.74
1:A:62:U:C2'	1:A:63:C:H5"	2.17	0.74
5:E:144:THR:HG22	5:E:147:ASP:OD2	1.87	0.74
6:F:48:LEU:HD13	6:F:52:ILE:HD12	1.70	0.74
7:G:75:VAL:HG12	7:G:76:ARG:H	1.53	0.74
12:L:47:LYS:CB	12:L:48:PRO:HD3	2.17	0.74
1:A:1366:C:H2'	1:A:1367:C:C6	2.23	0.73
6:F:69:GLU:O	6:F:72:VAL:HG23	1.88	0.73
7:G:12:LEU:H	7:G:12:LEU:HD12	1.53	0.73
1:A:1086:U:H3	1:A:1099:G:H22	1.35	0.73
1:A:523:A:N6	12:L:92:ASP:HB2	2.04	0.73
1:A:882:C:O2'	1:A:883:C:H5'	1.88	0.73
1:A:975:A:O5'	1:A:976:G:H5'	1.88	0.73
16:P:2:VAL:O	16:P:64:ALA:HA	1.88	0.73
2:B:19:HIS:CD2	2:B:20:GLU:HG2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:4:ILE:O	10:J:73:ASP:HA	1.87	0.73
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.70	0.73
13:M:22:ILE:HD12	13:M:25:ILE:HD12	1.69	0.73
1:A:107:G:C2'	1:A:108:G:H5'	2.18	0.73
1:A:474:G:N2	1:A:475:G:C4	2.56	0.73
1:A:254:G:OP1	17:Q:67:LYS:O	2.06	0.73
1:A:1447:G:O6	1:A:1460:A:N1	2.21	0.73
17:Q:24:GLU:HA	17:Q:39:SER:HB3	1.68	0.73
1:A:1060:C:H2'	1:A:1061:G:H8	1.53	0.73
1:A:1459:C:O5'	1:A:1459:C:H6	1.69	0.73
10:J:49:VAL:O	10:J:60:ARG:HA	1.89	0.73
1:A:1006:A:OP2	1:A:1006(A):C:H5"	1.89	0.73
1:A:504:C:H41	12:L:115:LYS:NZ	1.87	0.73
1:A:1372:U:O2'	1:A:1373:G:H5'	1.89	0.73
3:C:116:VAL:O	3:C:119:ARG:HB3	1.89	0.73
9:I:48:GLU:H	9:I:49:PRO:HD2	1.54	0.73
15:O:17:ARG:HG3	15:O:17:ARG:HH11	1.54	0.73
4:D:114:ARG:HH11	4:D:114:ARG:HG3	1.53	0.72
4:D:189:PRO:HB2	4:D:194:LEU:HD21	1.69	0.72
1:A:461:C:O2'	1:A:474:G:OP1	2.06	0.72
1:A:1064:G:C4'	1:A:1065:U:H5'	2.17	0.72
6:F:50:TYR:HE1	18:R:77:GLY:HA2	1.54	0.72
10:J:8:LEU:HD11	10:J:72:VAL:HG23	1.71	0.72
19:S:4:SER:O	19:S:5:LEU:HG	1.89	0.72
1:A:791:G:H2'	1:A:792:A:H5'	1.71	0.72
1:A:1015:A:H2'	1:A:1016:A:C8	2.23	0.72
1:A:1022:G:H2'	1:A:1023:G:H8	1.53	0.72
3:C:10:PHE:CE2	3:C:178:LEU:HD13	2.23	0.72
7:G:42:ILE:HG22	7:G:120:ILE:HD12	1.69	0.72
12:L:54:LYS:N	12:L:54:LYS:HD2	2.04	0.72
1:A:532:A:N7	3:C:161:GLU:HB2	2.04	0.72
4:D:62:GLN:HE22	4:D:65:ARG:NH1	1.88	0.72
1:A:976:G:N2	1:A:1362:C:H2'	2.04	0.72
10:J:38:ILE:HD11	10:J:71:LEU:CB	2.11	0.72
17:Q:95:TYR:HA	17:Q:98:LEU:HD11	1.72	0.72
1:A:530:G:N2	1:A:1492:A:H61	1.87	0.72
1:A:1498:U:H4'	1:A:1519:A:C2	2.24	0.72
3:C:43:LEU:HD11	3:C:68:VAL:HG22	1.71	0.72
3:C:59:ARG:H	10:J:92:THR:HG23	1.54	0.72
12:L:34:ARG:O	12:L:61:THR:HG23	1.90	0.72
12:L:53:ARG:HG2	12:L:53:ARG:HH11	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:83:VAL:HG23	12:L:107:ALA:HB2	1.71	0.72
1:A:1190:G:H3'	3:C:3:ASN:O	1.89	0.72
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.25	0.72
11:K:92:GLU:HA	11:K:95:ILE:HD12	1.72	0.72
1:A:590:C:OP1	8:H:30:ARG:HG2	1.89	0.72
1:A:1130:A:N6	1:A:1144:G:H21	1.86	0.72
6:F:14:LEU:HD21	6:F:18:GLN:HB2	1.70	0.72
11:K:87:THR:HG23	11:K:91:ARG:NH2	2.03	0.72
1:A:109:A:H2'	1:A:326:G:N2	2.05	0.71
1:A:149:A:H2'	1:A:150:C:H6	1.55	0.71
1:A:189:G:C2'	1:A:190:C:O5'	2.38	0.71
1:A:1003:G:C2'	1:A:1004:A:H5"	2.19	0.71
1:A:1191:A:H2'	1:A:1192:C:C6	2.24	0.71
2:B:58:ILE:HG23	2:B:68:ILE:CD1	2.21	0.71
13:M:25:ILE:HD11	13:M:60:VAL:HG13	1.72	0.71
1:A:91:C:H2'	1:A:92:C:H6	1.52	0.71
3:C:52:LEU:HG	3:C:118:GLN:HE22	1.55	0.71
14:N:45:ARG:HH11	14:N:45:ARG:HG3	1.55	0.71
1:A:107:G:H2'	1:A:108:G:H5'	1.72	0.71
12:L:28:LYS:C	12:L:30:ALA:H	1.91	0.71
1:A:555:C:H2'	1:A:556:C:H6	1.55	0.71
1:A:189:G:H2'	1:A:190:C:O5'	1.91	0.71
2:B:44:LEU:HA	2:B:47:THR:OG1	1.90	0.71
3:C:73:PRO:HA	3:C:76:VAL:HG21	1.71	0.71
2:B:45:GLN:CD	2:B:45:GLN:H	1.94	0.71
4:D:14:ARG:O	4:D:14:ARG:HD3	1.91	0.71
3:C:87:LEU:HA	3:C:90:GLU:HB3	1.73	0.71
4:D:160:GLN:O	4:D:163:GLU:HB3	1.89	0.71
13:M:9:ILE:HD12	13:M:9:ILE:N	2.06	0.71
2:B:178:ARG:HG3	2:B:178:ARG:NH1	2.05	0.71
11:K:34:ASP:HB2	11:K:35:PRO:HD2	1.73	0.71
11:K:43:SER:HB3	11:K:68:ALA:HB2	1.73	0.71
3:C:3:ASN:N	3:C:3:ASN:ND2	2.36	0.70
10:J:16:LEU:HD21	10:J:94:VAL:CG1	2.21	0.70
5:E:91:LEU:HD23	5:E:120:THR:HG22	1.72	0.70
16:P:26:ARG:HB3	16:P:26:ARG:HH11	1.56	0.70
1:A:35:G:H21	12:L:118:SER:CB	2.03	0.70
1:A:1123:A:C4'	10:J:37:PRO:HD2	2.20	0.70
2:B:236:TYR:O	2:B:239:VAL:HG23	1.90	0.70
7:G:64:GLN:HE21	7:G:68:ASN:ND2	1.89	0.70
15:O:87:ILE:HG22	15:O:88:ARG:HG2	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:U:H4'	1:A:1136:U:C5	2.26	0.70
12:L:46:LYS:HG2	12:L:47:LYS:H	1.57	0.70
12:L:47:LYS:HB2	12:L:48:PRO:CD	2.19	0.70
1:A:328:C:H4'	1:A:329:A:H5'	1.74	0.70
1:A:518:C:H4'	1:A:519:C:H6	1.57	0.70
1:A:1151:A:HO2'	1:A:1152:A:H8	1.37	0.70
1:A:1250:A:H4'	9:I:68:GLY:O	1.90	0.70
1:A:994:A:C8	1:A:1216:G:H4'	2.27	0.70
2:B:97:TRP:HZ2	2:B:102:LEU:CD1	2.04	0.70
12:L:89:ARG:NH2	12:L:97:ARG:HE	1.89	0.70
1:A:1489:G:H2'	1:A:1490:C:C5'	2.22	0.70
1:A:530:G:O6	22:X:3:G:C8	2.45	0.70
18:R:36:ASN:O	18:R:39:VAL:HG12	1.91	0.70
20:T:68:LYS:HE3	20:T:68:LYS:HA	1.72	0.70
1:A:1201:A:H4'	1:A:1202:G:O5'	1.92	0.70
2:B:81:VAL:HG12	2:B:92:TYR:HD1	1.57	0.70
1:A:188:C:H2'	1:A:189:G:H4'	1.72	0.70
1:A:190:C:C6	1:A:190:C:O5'	2.45	0.70
1:A:357:G:O2'	1:A:358:U:H5'	1.92	0.70
1:A:861:G:O2'	1:A:862:C:H5'	1.91	0.70
1:A:359:U:H2'	1:A:360:A:H8	1.55	0.69
2:B:18:GLY:CA	2:B:41:ILE:HA	2.22	0.69
2:B:212:GLN:HE22	2:B:235:SER:HB2	1.55	0.69
3:C:94:LEU:HD22	3:C:95:THR:HG23	1.73	0.69
8:H:14:ARG:HB3	8:H:14:ARG:HH11	1.57	0.69
5:E:91:LEU:CD2	5:E:120:THR:HG22	2.22	0.69
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.73	0.69
10:J:19:SER:O	10:J:23:ILE:HG13	1.92	0.69
19:S:62:ILE:HD12	19:S:66:MET:SD	2.32	0.69
1:A:191:G:H21	20:T:85:MET:CE	2.04	0.69
12:L:89:ARG:NH1	12:L:97:ARG:HG2	2.08	0.69
8:H:127:LEU:HD22	8:H:127:LEU:N	2.07	0.69
2:B:121:LEU:O	2:B:121:LEU:HD23	1.93	0.69
4:D:155:LEU:HB2	4:D:158:ILE:HD12	1.74	0.69
7:G:75:VAL:HG12	7:G:76:ARG:N	2.07	0.69
4:D:103:ASN:O	4:D:106:TYR:HB3	1.93	0.69
8:H:134:ILE:O	8:H:135:CYS:HB3	1.91	0.69
13:M:88:ARG:HG3	13:M:98:VAL:CG1	2.23	0.69
3:C:27:LYS:HB2	3:C:30:ARG:HH22	1.58	0.69
7:G:3:ARG:HG2	7:G:3:ARG:HH11	1.57	0.69
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:90:LEU:O	10:J:90:LEU:HD23	1.92	0.69
17:Q:48:GLU:O	17:Q:50:LYS:N	2.24	0.69
1:A:35:G:H2'	1:A:36:C:C6	2.27	0.69
1:A:188:C:C2'	1:A:189:G:H4'	2.23	0.69
1:A:427:U:H3'	1:A:428:G:H2'	1.74	0.69
1:A:797:C:O2'	1:A:798:G:H5'	1.92	0.69
1:A:1502:A:H2	1:A:1505:G:N1	1.91	0.69
2:B:87:ARG:O	2:B:87:ARG:HD2	1.93	0.69
2:B:112:VAL:HG22	2:B:149:LEU:HD13	1.74	0.69
6:F:68:PRO:HB2	6:F:71:ARG:HG3	1.72	0.69
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.28	0.69
16:P:1:MET:CE	16:P:3:LYS:HE3	2.23	0.69
1:A:523:A:H61	12:L:92:ASP:CB	2.05	0.69
1:A:592:G:O2'	1:A:593:G:H5'	1.93	0.69
1:A:1443:G:C4'	1:A:1446:A:H5'	2.23	0.69
2:B:15:VAL:HG12	2:B:210:SER:OG	1.93	0.69
8:H:19:VAL:CG2	8:H:21:LYS:HG3	2.23	0.69
1:A:575:G:OP1	1:A:575:G:H4'	1.93	0.68
1:A:640:A:O2'	1:A:641:U:H5'	1.94	0.68
1:A:1370:G:O2'	1:A:1371:G:H5'	1.92	0.68
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.74	0.68
7:G:15:ASP:HB3	7:G:19:GLY:H	1.57	0.68
1:A:112:G:N2	1:A:354:G:H5'	2.06	0.68
1:A:474:G:C5'	1:A:475:G:C8	2.77	0.68
1:A:1542:U:H2'	1:A:1543:C:O4'	1.94	0.68
2:B:217:ARG:HA	2:B:220:ASP:OD2	1.93	0.68
3:C:138:VAL:HG21	3:C:168:ALA:HB1	1.75	0.68
4:D:104:VAL:HG11	4:D:146:ILE:HD12	1.75	0.68
5:E:122:GLU:OE1	5:E:131:ILE:HG21	1.93	0.68
19:S:32:LYS:HA	19:S:50:ALA:O	1.92	0.68
1:A:442:C:C5	1:A:443:C:N4	2.62	0.68
6:F:35:ALA:HB1	6:F:65:VAL:HG11	1.74	0.68
1:A:253:U:H2'	1:A:254:G:C8	2.28	0.68
3:C:64:VAL:HB	3:C:99:VAL:HB	1.76	0.68
8:H:45:ILE:O	8:H:45:ILE:HG13	1.93	0.68
1:A:191:G:N2	20:T:85:MET:HE1	2.09	0.68
1:A:443:C:H2'	1:A:444:C:H6	1.59	0.68
2:B:92:TYR:HD2	2:B:151:GLY:HA3	1.57	0.68
1:A:911:U:H2'	1:A:912:C:C6	2.28	0.68
17:Q:5:VAL:HA	17:Q:59:ILE:O	1.94	0.68
1:A:76:C:N4	1:A:93:G:H22	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:U:O2'	1:A:63:C:H5"	1.92	0.68
5:E:103:GLY:O	5:E:106:PRO:HD2	1.92	0.68
1:A:718:G:C5'	11:K:117:ASN:HD22	2.07	0.68
2:B:139:LYS:C	2:B:139:LYS:HD3	2.15	0.68
3:C:23:TYR:OH	10:J:9:ARG:HD3	1.94	0.68
4:D:145:GLU:HG3	4:D:183:GLY:O	1.94	0.68
15:O:3:ILE:HD12	15:O:3:ILE:N	2.09	0.68
1:A:625:G:H2'	1:A:626:U:C6	2.30	0.67
1:A:723:U:O2	1:A:723:U:H2'	1.93	0.67
1:A:746:A:O2'	1:A:747:C:H5'	1.93	0.67
1:A:1539:C:O2	1:A:1539:C:H2'	1.94	0.67
3:C:6:HIS:CD2	3:C:8:ILE:H	2.11	0.67
1:A:191:G:C1'	20:T:105:SER:HA	2.23	0.67
1:A:530:G:H22	1:A:1492:A:H61	1.41	0.67
1:A:1490:C:H5'	1:A:1490:C:C6	2.18	0.67
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.57	0.67
1:A:1280:A:H5'	10:J:40:LEU:HD11	1.76	0.67
1:A:1475:G:H2'	1:A:1476:G:C8	2.29	0.67
1:A:1539:C:H41	7:G:81:GLY:C	1.97	0.67
8:H:86:ILE:HD11	8:H:136:GLU:HG3	1.76	0.67
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.10	0.67
15:O:6:GLU:H	15:O:6:GLU:CD	1.97	0.67
1:A:750:G:H1'	15:O:22:THR:OG1	1.95	0.67
1:A:1443:G:H5'	1:A:1447:G:OP1	1.94	0.67
2:B:142:LEU:HB3	2:B:146:GLN:HE21	1.59	0.67
2:B:187:LEU:HD22	2:B:201:ILE:O	1.95	0.67
4:D:150:GLU:H	4:D:150:GLU:CD	1.96	0.67
9:I:108:VAL:HG12	9:I:109:VAL:H	1.58	0.67
16:P:45:THR:HB	16:P:46:PRO:HD2	1.75	0.67
23:Y:38:A:H3'	23:Y:39:A:H5"	1.76	0.67
1:A:701:C:H5"	1:A:703:G:O4'	1.93	0.67
1:A:1004:A:H2'	1:A:1005:A:O4'	1.95	0.67
1:A:1147:C:H4'	9:I:5:TYR:CE1	2.30	0.67
2:B:16:HIS:CE1	2:B:210:SER:HB3	2.30	0.67
3:C:154:SER:O	3:C:157:ILE:HG13	1.94	0.67
9:I:19:LEU:HB3	9:I:59:PHE:CD2	2.30	0.67
1:A:1287:A:H2'	1:A:1288:A:C8	2.30	0.67
1:A:1343:G:H2'	1:A:1344:C:C6	2.30	0.67
1:A:1407:C:H2'	1:A:1408:A:H8	1.59	0.67
3:C:180:ALA:CB	3:C:182:ILE:HG13	2.25	0.67
4:D:64:LEU:HD12	4:D:75:PHE:HE1	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:89:ARG:CZ	12:L:97:ARG:HE	2.08	0.67
17:Q:68:ARG:HG3	17:Q:68:ARG:O	1.94	0.67
18:R:44:LEU:HD23	18:R:48:GLY:O	1.95	0.67
20:T:93:GLU:HA	20:T:93:GLU:OE2	1.94	0.67
1:A:1195:C:H3'	1:A:1196:U:H5'	1.76	0.67
1:A:1245:A:H61	1:A:1292:U:H3	1.42	0.67
3:C:90:GLU:HA	3:C:93:LYS:HG2	1.75	0.67
3:C:148:GLY:HA3	3:C:172:ARG:O	1.95	0.67
4:D:3:ARG:NE	4:D:118:ARG:HH11	1.93	0.67
4:D:117:ALA:O	4:D:121:VAL:HG23	1.95	0.67
8:H:127:LEU:H	8:H:127:LEU:CD2	2.08	0.67
1:A:1216:G:H5"	14:N:5:ALA:CB	2.21	0.67
1:A:1329:A:P	13:M:28:ALA:HB3	2.35	0.67
13:M:11:ARG:CZ	13:M:12:ASN:N	2.57	0.67
14:N:18:VAL:O	14:N:19:ARG:HG3	1.95	0.67
1:A:76:C:N4	1:A:93:G:H1	1.93	0.67
1:A:518:C:H2'	1:A:530:G:N3	2.10	0.67
1:A:707:C:H2'	1:A:708:C:H6	1.60	0.67
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.75	0.67
3:C:19:GLU:HB3	3:C:40:ARG:NH2	2.10	0.66
3:C:179:ARG:NH1	3:C:206:GLU:HG2	2.09	0.66
4:D:150:GLU:HA	4:D:153:ARG:HE	1.60	0.66
9:I:108:VAL:HG12	9:I:109:VAL:N	2.10	0.66
11:K:29:ILE:HG22	11:K:44:SER:HB2	1.76	0.66
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.77	0.66
13:M:11:ARG:HA	13:M:11:ARG:HH11	1.59	0.66
18:R:55:ARG:NH1	18:R:55:ARG:HB3	2.10	0.66
1:A:1030:C:H2'	1:A:1030(A):G:N7	2.10	0.66
8:H:107:LEU:HD23	8:H:107:LEU:N	2.10	0.66
19:S:42:PRO:O	19:S:45:VAL:HG23	1.95	0.66
1:A:168:G:O2'	1:A:169:C:H5'	1.96	0.66
1:A:1318:A:H4'	19:S:10:PHE:CE2	2.30	0.66
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.09	0.66
1:A:406:G:H5"	4:D:5:ILE:HG23	1.77	0.66
4:D:189:PRO:HB2	4:D:194:LEU:CD2	2.25	0.66
1:A:77:G:O2'	1:A:78:G:H5'	1.95	0.66
1:A:189:G:N2	1:A:190:C:H1'	2.11	0.66
1:A:909:A:H2'	1:A:910:C:O4'	1.95	0.66
1:A:1152:A:H5'	10:J:70:ARG:NH2	2.09	0.66
1:A:1223:C:P	19:S:78:ARG:HH12	2.19	0.66
3:C:19:GLU:HB3	3:C:40:ARG:HH21	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:39:VAL:HG13	18:R:40:LEU:N	2.10	0.66
1:A:664:G:H22	1:A:741:G:H1	1.43	0.66
1:A:973:G:H3'	1:A:974:A:H5"	1.76	0.66
1:A:1006:A:OP1	1:A:1038:C:H4'	1.96	0.66
2:B:136:VAL:O	2:B:140:HIS:HB2	1.95	0.66
4:D:59:ARG:NE	4:D:59:ARG:HA	2.11	0.66
1:A:458:C:O2	1:A:458:C:H2'	1.94	0.66
1:A:620:C:N1	4:D:135:LEU:HD13	2.10	0.66
1:A:1202:G:H2'	1:A:1203:C:O4'	1.95	0.66
1:A:443:C:H2'	1:A:444:C:C6	2.30	0.66
1:A:1007:C:H2'	1:A:1008:C:C6	2.30	0.66
2:B:24:TRP:HD1	2:B:24:TRP:H	1.43	0.66
10:J:40:LEU:HD12	10:J:41:PRO:HD2	1.77	0.66
10:J:59:SER:O	10:J:60:ARG:HB2	1.95	0.66
1:A:393:A:O2'	1:A:394:G:H5'	1.95	0.66
1:A:1495:U:H2'	1:A:1496:C:H6	1.61	0.66
2:B:25:ASN:HD22	2:B:25:ASN:C	1.98	0.66
8:H:14:ARG:HH11	8:H:14:ARG:CB	2.09	0.66
8:H:112:LEU:HD23	8:H:112:LEU:H	1.61	0.66
10:J:55:LYS:O	10:J:56:HIS:HB2	1.96	0.66
1:A:707:C:H2'	1:A:708:C:C6	2.30	0.65
3:C:88:ARG:HA	3:C:101:LEU:HD12	1.78	0.65
12:L:93:LEU:HD12	12:L:96:VAL:HG21	1.78	0.65
1:A:384:G:H2'	1:A:385:C:C6	2.32	0.65
2:B:97:TRP:HZ3	2:B:99:GLY:HA2	1.61	0.65
11:K:17:GLY:O	11:K:80:VAL:HA	1.96	0.65
13:M:66:LEU:H	13:M:66:LEU:HD12	1.61	0.65
15:O:10:LYS:HD2	15:O:10:LYS:C	2.16	0.65
1:A:269:C:H2'	1:A:270:A:H8	1.61	0.65
1:A:1288:A:H2'	1:A:1289:A:H8	1.62	0.65
17:Q:80:GLY:O	17:Q:81:ARG:HB3	1.97	0.65
1:A:542:G:OP1	4:D:10:ARG:NH2	2.28	0.65
1:A:839:U:H5'	1:A:840:C:H5	1.60	0.65
1:A:1426:C:H2'	1:A:1427:U:C6	2.30	0.65
1:A:1477:C:H2'	1:A:1478:C:H6	1.62	0.65
2:B:55:PHE:HD2	2:B:58:ILE:HD12	1.61	0.65
4:D:187:ARG:HD2	4:D:188:LEU:H	1.62	0.65
1:A:434:U:H2'	1:A:435:C:C6	2.31	0.65
1:A:919:A:O2'	1:A:920:U:H5'	1.97	0.65
7:G:15:ASP:HB3	7:G:19:GLY:N	2.10	0.65
8:H:69:ARG:HG2	8:H:70:GLN:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:U:H4'	9:I:14:VAL:HG11	1.77	0.65
17:Q:18:THR:OG1	17:Q:69:LYS:HE3	1.97	0.65
17:Q:40:LYS:HD2	17:Q:42:TYR:CE1	2.31	0.65
1:A:332:G:OP2	20:T:10:LEU:HG	1.97	0.65
1:A:1191:A:H5"	3:C:4:LYS:HE3	1.79	0.65
3:C:187:ALA:HB3	3:C:198:VAL:HB	1.79	0.65
8:H:11:THR:HA	8:H:14:ARG:HH12	1.62	0.65
10:J:89:ASP:HB2	10:J:91:PRO:HD2	1.79	0.65
20:T:43:LEU:HD13	20:T:51:GLU:HG3	1.79	0.65
1:A:502:G:H4'	1:A:550:G:H4'	1.78	0.65
1:A:1095:U:H2'	1:A:1096:C:C6	2.31	0.65
19:S:49:ILE:O	19:S:60:VAL:HB	1.96	0.65
1:A:633:G:H2'	1:A:634:C:C6	2.32	0.65
1:A:918:A:H2'	1:A:919:A:H8	1.57	0.65
1:A:1241:G:H2'	1:A:1242:C:C6	2.31	0.65
10:J:53:PRO:HA	14:N:41:ARG:NH2	2.11	0.65
1:A:1372:U:OP1	9:I:71:SER:HB3	1.96	0.65
3:C:110:ASN:ND2	3:C:140:ARG:HD3	2.12	0.65
1:A:1047:G:O2'	1:A:1048:G:H5'	1.98	0.64
4:D:126:ILE:HG22	4:D:127:THR:N	2.11	0.64
8:H:10:LEU:CD2	8:H:83:ILE:HD11	2.27	0.64
9:I:127:LYS:HD2	9:I:127:LYS:N	2.12	0.64
10:J:16:LEU:HA	10:J:19:SER:HB3	1.79	0.64
12:L:33:ARG:HG2	12:L:60:LEU:HD12	1.77	0.64
13:M:48:LEU:HB3	13:M:53:VAL:HG23	1.80	0.64
13:M:49:THR:HG22	13:M:51:ALA:H	1.61	0.64
19:S:32:LYS:HB3	19:S:50:ALA:HB3	1.80	0.64
1:A:403:C:H4'	4:D:122:ARG:NH1	2.12	0.64
1:A:839:U:H5'	1:A:840:C:C5	2.32	0.64
1:A:1104:G:H4'	2:B:111:ARG:NH2	2.12	0.64
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.79	0.64
9:I:11:LYS:O	9:I:11:LYS:HG2	1.97	0.64
9:I:85:LEU:HB3	9:I:92:TYR:HD1	1.62	0.64
1:A:1060:C:O2'	10:J:56:HIS:HD2	1.81	0.64
3:C:26:LYS:HE2	3:C:26:LYS:N	2.12	0.64
1:A:19:C:H2'	1:A:20:U:H6	1.62	0.64
1:A:838:G:C2'	1:A:839:U:H5"	2.28	0.64
1:A:1003:G:H2'	1:A:1004:A:C5'	2.27	0.64
1:A:22:G:H2'	1:A:23:C:C6	2.33	0.64
1:A:394:G:H2'	1:A:395:C:C6	2.33	0.64
1:A:530:G:O6	22:X:3:G:H8	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1499:A:O2'	1:A:1500:A:H5'	1.97	0.64
5:E:107:ARG:HG2	5:E:108:ALA:N	2.11	0.64
10:J:26:ALA:HB1	10:J:30:SER:OG	1.96	0.64
12:L:38:THR:HG22	12:L:39:VAL:HG13	1.80	0.64
5:E:9:LYS:CD	5:E:112:LEU:HD21	2.27	0.64
7:G:22:LEU:O	7:G:22:LEU:HD23	1.96	0.64
12:L:28:LYS:C	12:L:30:ALA:N	2.50	0.64
14:N:14:PRO:HG2	14:N:15:LYS:H	1.62	0.64
16:P:74:LEU:O	16:P:79:VAL:HG23	1.97	0.64
20:T:67:ALA:HA	20:T:73:HIS:H	1.63	0.64
1:A:269:C:H2'	1:A:270:A:C8	2.33	0.64
1:A:1022:G:H2'	1:A:1023:G:C8	2.33	0.64
1:A:1331:G:OP1	1:A:1331:G:H4'	1.98	0.64
17:Q:36:ILE:H	17:Q:36:ILE:HD13	1.63	0.64
1:A:191:G:C8	1:A:191:G:H5"	2.33	0.64
1:A:349:A:H2'	1:A:350:G:H5"	1.80	0.64
1:A:533:A:O2'	1:A:534:U:OP1	2.16	0.64
1:A:1195:C:H3'	1:A:1196:U:C5'	2.27	0.64
1:A:1263:C:H2'	1:A:1264:C:C6	2.33	0.64
1:A:1475:G:H2'	1:A:1476:G:H8	1.62	0.64
4:D:108:LEU:HB3	4:D:110:PHE:HE1	1.62	0.64
13:M:120:LYS:HG2	13:M:121:LYS:H	1.62	0.64
16:P:40:ASP:HB3	16:P:48:TRP:HB2	1.80	0.64
1:A:474:G:H5'	1:A:475:G:C8	2.33	0.64
1:A:522:C:H41	12:L:53:ARG:NH2	1.89	0.64
1:A:977:A:H2'	1:A:978:A:H5"	1.79	0.64
1:A:991:U:H5'	1:A:992:U:OP1	1.97	0.64
1:A:1288:A:H2'	1:A:1289:A:C8	2.32	0.64
3:C:14:ILE:HG22	3:C:15:THR:N	2.13	0.64
1:A:474:G:O5'	1:A:474:G:C4	2.51	0.64
1:A:1135:U:O2'	1:A:1136:U:H2'	1.97	0.64
1:A:1510:U:H2'	1:A:1511:G:C8	2.33	0.64
2:B:23:ARG:O	2:B:23:ARG:HD3	1.98	0.64
4:D:35:ARG:O	4:D:36:ARG:HG3	1.98	0.64
23:Y:34:C:H2'	23:Y:34:C:O2	1.97	0.64
1:A:99:C:H2'	1:A:101:A:O4'	1.97	0.63
1:A:405:U:H3'	1:A:406:G:H5'	1.79	0.63
1:A:1405:G:H2'	1:A:1406:U:H6	1.63	0.63
3:C:74:GLY:C	3:C:76:VAL:H	2.02	0.63
5:E:80:ILE:CD1	5:E:91:LEU:HD12	2.28	0.63
10:J:49:VAL:CG1	14:N:41:ARG:HD2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:56:ALA:O	12:L:58:VAL:HG23	1.98	0.63
19:S:77:THR:HG23	19:S:78:ARG:H	1.62	0.63
1:A:1443:G:H5"	1:A:1446:A:H5'	1.79	0.63
5:E:80:ILE:HD11	5:E:91:LEU:HD12	1.81	0.63
9:I:65:VAL:HG11	9:I:77:ILE:HD11	1.80	0.63
1:A:371:G:O2'	1:A:372:C:H5'	1.98	0.63
1:A:377:G:OP1	16:P:3:LYS:NZ	2.32	0.63
1:A:1129:C:H1'	1:A:1132:C:C5	2.29	0.63
1:A:1353:G:O2'	1:A:1354:C:H5'	1.98	0.63
2:B:213:LEU:HD23	2:B:213:LEU:C	2.17	0.63
9:I:79:LEU:CD1	9:I:83:ARG:HD2	2.27	0.63
1:A:1437:C:H2'	1:A:1438:G:H8	1.64	0.63
3:C:91:LEU:HD23	3:C:92:ALA:N	2.13	0.63
1:A:180:U:H2'	1:A:181:G:H5'	1.79	0.63
1:A:188:C:H2'	1:A:189:G:C4'	2.28	0.63
1:A:1281:U:H5'	1:A:1282:C:H5	1.64	0.63
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.34	0.63
3:C:7:PRO:CG	3:C:184:TYR:HB2	2.28	0.63
4:D:128:VAL:C	4:D:129:ASN:HD22	2.02	0.63
13:M:25:ILE:HG13	13:M:66:LEU:HD23	1.80	0.63
1:A:1006:A:P	1:A:1006(A):C:H5"	2.39	0.63
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.14	0.63
4:D:128:VAL:HG12	4:D:129:ASN:ND2	2.14	0.63
9:I:63:ILE:HG22	9:I:65:VAL:H	1.64	0.63
12:L:26:ALA:O	12:L:27:LEU:O	2.17	0.63
1:A:21:G:H2'	1:A:22:G:C8	2.34	0.63
1:A:32:A:H2'	1:A:33:A:C8	2.33	0.63
1:A:299:G:H2'	1:A:300:A:C8	2.34	0.63
1:A:397:A:H5'	1:A:398:C:OP1	1.99	0.63
1:A:1058:G:H2'	1:A:1059:C:O4'	1.99	0.63
3:C:180:ALA:HB3	3:C:182:ILE:HG13	1.80	0.63
7:G:101:LEU:O	7:G:104:LEU:HB2	1.99	0.63
7:G:144:MET:O	7:G:147:ALA:HB3	1.98	0.63
11:K:43:SER:CB	11:K:68:ALA:HB2	2.29	0.63
19:S:77:THR:HG23	19:S:78:ARG:N	2.12	0.63
1:A:1280:A:C5'	10:J:40:LEU:HD11	2.29	0.63
1:A:1539:C:N4	7:G:81:GLY:O	2.32	0.63
2:B:12:GLU:C	2:B:14:GLY:H	2.02	0.63
4:D:8:VAL:HG22	4:D:115:ARG:CZ	2.28	0.63
9:I:110:GLU:HG2	9:I:113:LYS:NZ	2.14	0.63
10:J:42:THR:HG23	10:J:67:THR:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:A:H1'	1:A:222:U:O2'	1.98	0.62
1:A:474:G:N3	1:A:474:G:C5'	2.61	0.62
1:A:1443:G:C5'	1:A:1446:A:H5'	2.29	0.62
3:C:10:PHE:CD2	3:C:178:LEU:HD13	2.34	0.62
8:H:11:THR:HA	8:H:14:ARG:NH1	2.14	0.62
20:T:91:LEU:C	20:T:93:GLU:H	2.00	0.62
5:E:32:VAL:HG12	5:E:58:ALA:HB1	1.81	0.62
8:H:68:ARG:HG2	8:H:68:ARG:HH11	1.63	0.62
13:M:54:VAL:O	13:M:58:GLU:HG2	1.99	0.62
20:T:102:GLY:O	20:T:104:LEU:N	2.31	0.62
2:B:102:LEU:HD21	2:B:162:ILE:CD1	2.28	0.62
7:G:32:ARG:C	7:G:34:GLY:H	2.03	0.62
7:G:107:ALA:C	7:G:109:ASN:H	2.03	0.62
16:P:1:MET:HE3	16:P:3:LYS:HE3	1.80	0.62
2:B:151:GLY:C	2:B:153:ARG:N	2.51	0.62
2:B:169:LYS:O	2:B:169:LYS:HD3	1.99	0.62
3:C:191:THR:CG2	3:C:192:THR:N	2.56	0.62
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.32	0.62
19:S:40:ILE:HG21	19:S:62:ILE:HD11	1.81	0.62
1:A:76:C:H42	1:A:93:G:H22	1.46	0.62
1:A:1251:A:H2'	1:A:1252:A:C8	2.35	0.62
1:A:1539:C:N4	7:G:81:GLY:C	2.53	0.62
3:C:59:ARG:H	10:J:92:THR:CG2	2.12	0.62
12:L:28:LYS:O	12:L:30:ALA:N	2.32	0.62
1:A:1003:G:C3'	1:A:1004:A:H5"	2.29	0.62
2:B:75:LYS:O	2:B:75:LYS:HD3	1.99	0.62
4:D:13:ARG:HD3	4:D:36:ARG:HB3	1.82	0.62
7:G:116:ALA:CA	7:G:119:ARG:HH21	2.12	0.62
1:A:191:G:H2'	1:A:192:U:O5'	1.99	0.62
1:A:1066:C:O2'	1:A:1067:A:H5'	2.00	0.62
1:A:1397:C:H4'	1:A:1398:A:OP2	1.98	0.62
19:S:14:HIS:O	19:S:18:LYS:HE3	2.00	0.62
1:A:968:A:C8	1:A:1062:U:H4'	2.35	0.62
1:A:1125:U:H5"	1:A:1126:U:O4	1.99	0.62
1:A:1193:G:O2'	1:A:1194:U:H5'	1.99	0.62
19:S:16:LEU:O	19:S:20:LEU:HG	2.00	0.62
1:A:737:A:H2'	1:A:738:C:C6	2.35	0.62
1:A:1006(A):C:H3'	1:A:1007:C:H6	1.65	0.62
1:A:1316:G:N2	1:A:1318:A:H3'	2.14	0.62
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.82	0.62
5:E:31:LEU:CD1	5:E:43:LEU:HD21	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:29:ARG:HD2	19:S:29:ARG:N	2.15	0.62
1:A:972:C:H4'	10:J:57:LYS:CG	2.26	0.62
3:C:34:LEU:HG	14:N:25:VAL:HG21	1.81	0.62
5:E:51:VAL:HB	5:E:52:PRO:CD	2.24	0.62
12:L:46:LYS:CG	12:L:47:LYS:H	2.13	0.62
1:A:1402:C:H2'	1:A:1403:C:O4'	2.00	0.61
5:E:100:VAL:O	5:E:107:ARG:NH2	2.33	0.61
7:G:64:GLN:HE21	7:G:68:ASN:HD21	1.47	0.61
1:A:335:C:O2'	1:A:336:C:H5'	2.00	0.61
1:A:718:G:C4'	11:K:117:ASN:HD22	2.13	0.61
1:A:1250:A:H2'	1:A:1251:A:H8	1.65	0.61
4:D:64:LEU:O	4:D:64:LEU:HD13	1.99	0.61
21:V:13:ILE:O	21:V:16:GLY:N	2.26	0.61
1:A:188:C:C3'	1:A:189:G:H4'	2.31	0.61
1:A:1286:A:C8	1:A:1287:A:H4'	2.35	0.61
2:B:90:MET:HE3	2:B:222:ILE:HD13	1.82	0.61
2:B:91:PRO:HG3	2:B:154:LEU:HG	1.82	0.61
5:E:36:ASP:O	5:E:37:ARG:HB2	1.99	0.61
6:F:53:ALA:O	6:F:54:LYS:HB2	2.00	0.61
1:A:718:G:H5'	11:K:117:ASN:HD22	1.64	0.61
1:A:718:G:H4'	11:K:117:ASN:ND2	2.16	0.61
1:A:1145:C:H1'	1:A:1146:A:N7	2.14	0.61
1:A:1544:U:O3'	22:X:1:C:OP1	2.09	0.61
10:J:77:PRO:HA	10:J:82:ILE:HD11	1.82	0.61
11:K:126:ARG:NH2	11:K:129:SER:HB3	2.14	0.61
1:A:191:G:H5"	1:A:191:G:H8	1.65	0.61
1:A:253:U:H2'	1:A:254:G:H8	1.65	0.61
1:A:1366:C:O2'	1:A:1367:C:H5'	2.01	0.61
2:B:162:ILE:CG2	2:B:164:VAL:HG23	2.31	0.61
7:G:149:ARG:O	7:G:149:ARG:HD2	2.00	0.61
10:J:82:ILE:HG22	10:J:82:ILE:O	1.99	0.61
12:L:35:GLY:HA3	12:L:58:VAL:CG1	2.31	0.61
17:Q:21:VAL:HG21	17:Q:59:ILE:HD11	1.81	0.61
3:C:83:ARG:C	3:C:85:ARG:H	2.03	0.61
7:G:21:VAL:C	7:G:23:VAL:H	2.04	0.61
15:O:66:LEU:O	15:O:69:TYR:HB3	2.01	0.61
1:A:946:A:H2'	1:A:947:G:C8	2.35	0.61
1:A:1145:C:H1'	1:A:1146:A:C8	2.36	0.61
1:A:1406:U:C2'	1:A:1407:C:H5'	2.30	0.61
3:C:174:PRO:O	3:C:177:THR:HG22	2.01	0.61
4:D:64:LEU:HD12	4:D:75:PHE:CE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:ILE:HG23	5:E:142:LEU:HD13	1.82	0.61
7:G:42:ILE:HG22	7:G:120:ILE:CD1	2.30	0.61
11:K:20:TYR:HD2	11:K:83:ILE:HB	1.65	0.61
11:K:121:PRO:HG2	11:K:126:ARG:CG	2.30	0.61
1:A:328:C:O2	1:A:328:C:H2'	2.00	0.61
1:A:1020:U:H2'	1:A:1021:G:C8	2.36	0.61
3:C:22:TRP:HA	10:J:93:GLY:CA	2.30	0.61
6:F:86:ARG:O	6:F:87:ARG:HG2	2.00	0.61
10:J:12:ASP:HB3	10:J:15:THR:CG2	2.30	0.61
1:A:633:G:H2'	1:A:634:C:H6	1.66	0.61
1:A:1249:C:C2'	1:A:1250:A:H5'	2.30	0.61
1:A:1435:G:H2'	1:A:1436:U:H6	1.63	0.61
2:B:8:LYS:HG3	2:B:48:MET:HE3	1.83	0.61
2:B:80:ILE:HG23	2:B:212:GLN:NE2	2.05	0.61
3:C:145:GLY:O	3:C:146:ALA:HB3	2.01	0.61
1:A:403:C:O2'	1:A:404:U:H5'	2.01	0.61
1:A:1171:G:H2'	1:A:1172:C:C6	2.36	0.61
3:C:179:ARG:HH11	3:C:206:GLU:CG	2.14	0.61
3:C:179:ARG:HD2	3:C:179:ARG:O	2.01	0.61
12:L:36:VAL:O	12:L:37:CYS:CB	2.49	0.61
13:M:79:LYS:O	13:M:79:LYS:HD3	2.00	0.61
1:A:188:C:C2	1:A:189:G:H1'	2.36	0.60
1:A:189:G:N3	1:A:190:C:H1'	2.16	0.60
1:A:474:G:H5"	1:A:475:G:C8	2.36	0.60
1:A:960:U:O2	1:A:960:U:H2'	2.00	0.60
1:A:1487:G:O2'	1:A:1488:G:H5'	2.01	0.60
4:D:79:PHE:HE1	4:D:204:ILE:HG12	1.66	0.60
7:G:71:PRO:O	7:G:96:GLN:HG3	2.01	0.60
8:H:69:ARG:NH1	8:H:75:ARG:O	2.34	0.60
12:L:60:LEU:HD23	12:L:64:TYR:O	2.00	0.60
13:M:14:ARG:HG3	13:M:44:ARG:NH2	2.16	0.60
13:M:87:TYR:C	13:M:89:GLY:H	2.05	0.60
1:A:285:G:O2'	1:A:286:G:H5'	2.01	0.60
1:A:492:G:H2'	1:A:494:G:H8	1.66	0.60
1:A:1505:G:H2'	1:A:1541:U:OP2	2.01	0.60
1:A:1527:C:O2'	1:A:1528:U:H5'	2.01	0.60
2:B:55:PHE:HA	2:B:58:ILE:HD12	1.84	0.60
3:C:73:PRO:O	3:C:76:VAL:HB	2.01	0.60
8:H:84:ARG:HD3	8:H:136:GLU:OE1	2.01	0.60
14:N:36:PHE:O	14:N:36:PHE:CD1	2.55	0.60
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:20:LEU:HA	19:S:23:ASN:HD22	1.64	0.60
1:A:282:A:C4	1:A:283:C:C6	2.90	0.60
1:A:1201:A:H4'	1:A:1202:G:C5'	2.31	0.60
9:I:65:VAL:CG2	9:I:73:GLN:HB3	2.31	0.60
13:M:117:VAL:HG23	13:M:118:ALA:N	2.12	0.60
1:A:447:G:H2'	1:A:485:G:H22	1.64	0.60
1:A:491:G:H2'	1:A:492:G:H8	1.66	0.60
1:A:706:A:O2'	11:K:29:ILE:HD11	2.02	0.60
1:A:1072:G:H2'	1:A:1073:U:C6	2.36	0.60
3:C:195:VAL:C	3:C:196:LEU:HD23	2.21	0.60
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.84	0.60
6:F:37:VAL:O	6:F:38:GLU:HG3	2.01	0.60
1:A:314:C:O2'	1:A:315:A:H5'	2.01	0.60
1:A:455:C:N4	1:A:477:G:H1	1.91	0.60
3:C:15:THR:O	3:C:16:ARG:HB2	2.00	0.60
16:P:52:ASP:O	16:P:52:ASP:OD1	2.18	0.60
4:D:64:LEU:HD11	4:D:97:LEU:CD1	2.32	0.60
4:D:108:LEU:O	4:D:176:LEU:HD22	2.02	0.60
11:K:14:VAL:O	11:K:15:ALA:HB3	2.01	0.60
11:K:54:ARG:HA	11:K:57:THR:HG23	1.83	0.60
21:V:2:GLY:O	21:V:4:GLY:N	2.35	0.60
1:A:933:G:OP2	7:G:3:ARG:HB2	2.02	0.60
1:A:1176:A:H2'	1:A:1177:G:C8	2.37	0.60
1:A:1218:C:H2'	1:A:1219:U:C6	2.36	0.60
10:J:4:ILE:HG21	10:J:74:ILE:HD12	1.84	0.60
14:N:8:GLU:O	14:N:11:LYS:HG3	2.02	0.60
1:A:36:C:C2'	1:A:37:U:H5'	2.31	0.60
1:A:92:C:H2'	1:A:93:G:C8	2.36	0.60
1:A:232:G:H1'	1:A:262:A:N1	2.17	0.60
1:A:352:C:H4'	1:A:354:G:OP1	2.01	0.60
6:F:91:VAL:HG21	18:R:72:ARG:CZ	2.32	0.60
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.84	0.60
9:I:60:ASP:O	9:I:61:ALA:HB2	2.00	0.60
12:L:93:LEU:N	12:L:93:LEU:CD2	2.64	0.60
17:Q:8:GLY:HA3	17:Q:22:LEU:O	2.00	0.60
1:A:1237:C:H4'	1:A:1334:G:N2	2.17	0.60
1:A:1379:G:N7	7:G:2:ALA:HB3	2.17	0.60
2:B:108:ILE:O	2:B:108:ILE:HG22	2.00	0.60
4:D:25:ARG:C	4:D:27:TYR:H	2.04	0.60
9:I:65:VAL:HG13	9:I:65:VAL:O	2.01	0.60
19:S:28:LYS:HG2	19:S:29:ARG:N	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1490:C:O2'	1:A:1491:G:H5'	2.01	0.60
2:B:142:LEU:HB3	2:B:146:GLN:NE2	2.16	0.60
3:C:17:ASP:OD1	3:C:18:TRP:N	2.35	0.60
11:K:19:ALA:HB2	11:K:80:VAL:HG11	1.84	0.60
11:K:40:ILE:HG22	11:K:41:THR:N	2.16	0.60
1:A:677:U:H3	1:A:713:G:H22	1.48	0.59
1:A:1257:U:H4'	1:A:1258:G:O5'	2.03	0.59
1:A:1277:C:H1'	1:A:1282:C:O2	2.01	0.59
3:C:191:THR:HG21	3:C:193:TYR:CE2	2.37	0.59
4:D:36:ARG:HG2	4:D:38:TYR:CE1	2.36	0.59
12:L:71:PRO:O	12:L:102:ARG:HD2	2.02	0.59
13:M:23:TYR:CD2	13:M:70:LEU:HD13	2.37	0.59
20:T:56:MET:HE3	20:T:88:VAL:HG11	1.83	0.59
1:A:410:G:OP2	4:D:25:ARG:HD2	2.03	0.59
1:A:780:A:O2'	1:A:781:A:H5"	2.02	0.59
1:A:1090:U:H2'	1:A:1091:U:H6	1.67	0.59
12:L:47:LYS:CB	12:L:48:PRO:CD	2.77	0.59
13:M:24:GLY:HA3	13:M:66:LEU:HB3	1.84	0.59
13:M:97:PRO:HB2	13:M:101:GLN:OE1	2.03	0.59
1:A:740:U:O2'	1:A:741:G:H5'	2.03	0.59
1:A:983:A:H5'	1:A:984:C:OP2	2.01	0.59
1:A:1152:A:H5'	10:J:70:ARG:HH22	1.66	0.59
1:A:1260:C:O5'	1:A:1284:C:H4'	2.02	0.59
1:A:1497:G:C2'	1:A:1498:U:H5'	2.32	0.59
3:C:108:ASN:C	3:C:110:ASN:H	2.05	0.59
5:E:12:LEU:HD13	5:E:31:LEU:HB3	1.84	0.59
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.36	0.59
1:A:216:G:H2'	1:A:217:C:O4'	2.03	0.59
1:A:792:A:H4'	1:A:793:U:H5"	1.83	0.59
4:D:110:PHE:CD1	4:D:110:PHE:N	2.68	0.59
6:F:38:GLU:HB2	6:F:64:GLN:O	2.02	0.59
9:I:28:VAL:HG21	9:I:33:PHE:HD1	1.67	0.59
13:M:91:ARG:HB2	13:M:98:VAL:HG22	1.84	0.59
20:T:50:GLU:O	20:T:100:ILE:HD12	2.02	0.59
1:A:308:C:H2'	1:A:309:G:C8	2.38	0.59
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.37	0.59
3:C:153:VAL:HG12	3:C:154:SER:N	2.15	0.59
7:G:38:LEU:O	7:G:42:ILE:HG13	2.02	0.59
7:G:90:GLU:H	7:G:155:ARG:NH2	1.96	0.59
7:G:111:ARG:HH11	7:G:111:ARG:CB	2.08	0.59
9:I:11:LYS:O	9:I:12:GLU:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:24:VAL:HG21	10:J:72:VAL:HG13	1.85	0.59
12:L:83:VAL:HG22	12:L:84:LEU:N	2.18	0.59
1:A:490:G:O2'	1:A:491:G:H5'	2.03	0.59
1:A:1189:C:P	10:J:51:ARG:HH22	2.25	0.59
2:B:9:GLU:OE2	2:B:12:GLU:HA	2.02	0.59
5:E:31:LEU:HD23	5:E:45:PHE:CD1	2.37	0.59
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.85	0.59
7:G:105:VAL:HA	7:G:108:ALA:HB3	1.85	0.59
13:M:22:ILE:HG21	13:M:66:LEU:HD22	1.84	0.59
1:A:439:A:H5"	1:A:494:G:H22	1.66	0.59
1:A:1152:A:H5"	10:J:13:HIS:HB2	1.85	0.59
1:A:1436:U:H2'	1:A:1437:C:H6	1.67	0.59
6:F:35:ALA:HA	6:F:67:MET:HB3	1.84	0.59
7:G:26:PHE:HB2	7:G:62:PHE:HZ	1.68	0.59
10:J:55:LYS:HG3	10:J:56:HIS:ND1	2.18	0.59
13:M:6:GLY:O	13:M:8:GLU:N	2.30	0.59
1:A:252:U:H2'	1:A:253:U:C6	2.38	0.59
1:A:337:C:H2'	1:A:338:A:H8	1.68	0.59
1:A:411:A:C1'	1:A:413:G:H1'	2.33	0.59
1:A:1090:U:O2'	1:A:1091:U:H5'	2.03	0.59
2:B:95:GLN:C	2:B:96:ARG:HD2	2.23	0.59
3:C:81:GLY:HA2	3:C:84:ILE:HG22	1.85	0.59
10:J:15:THR:O	10:J:19:SER:HB2	2.02	0.59
10:J:49:VAL:CG1	14:N:41:ARG:HB2	2.33	0.59
11:K:33:THR:HA	11:K:39:PRO:HA	1.84	0.59
13:M:11:ARG:NH1	13:M:12:ASN:H	2.01	0.59
13:M:44:ARG:HB3	13:M:46:LYS:HG2	1.83	0.59
13:M:97:PRO:N	13:M:110:ARG:HG2	2.18	0.59
16:P:40:ASP:HB3	16:P:48:TRP:CB	2.33	0.59
1:A:189:G:N3	1:A:190:C:C1'	2.66	0.59
1:A:828:A:H2'	1:A:829:G:O4'	2.03	0.59
2:B:101:MET:N	2:B:108:ILE:HD12	2.18	0.59
3:C:84:ILE:O	3:C:88:ARG:HD2	2.03	0.59
3:C:155:GLY:O	3:C:156:ARG:C	2.41	0.59
7:G:72:ARG:O	7:G:73:MET:HG2	2.03	0.59
14:N:3:ARG:HD3	14:N:6:LEU:HD12	1.85	0.59
2:B:69:LEU:HD23	2:B:69:LEU:C	2.23	0.58
8:H:104:ARG:NH2	8:H:138:TRP:CH2	2.71	0.58
13:M:44:ARG:HG2	13:M:46:LYS:HE3	1.83	0.58
18:R:29:PHE:HE1	18:R:31:LEU:HD23	1.68	0.58
19:S:26:GLY:O	19:S:27:GLU:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:ASN:ND2	3:C:3:ASN:H	2.00	0.58
3:C:157:ILE:HD12	3:C:164:ARG:HG3	1.85	0.58
12:L:24:VAL:O	12:L:24:VAL:HG12	2.03	0.58
15:O:64:ARG:HH11	15:O:64:ARG:HG3	1.68	0.58
1:A:33:A:H2'	1:A:34:C:C6	2.38	0.58
2:B:132:LYS:HA	2:B:135:GLN:HB3	1.85	0.58
12:L:111:LYS:O	12:L:112:ASP:HB2	2.04	0.58
12:L:117:ARG:NH2	12:L:124:LYS:HA	2.18	0.58
13:M:40:ASN:HD22	13:M:41:PRO:N	2.00	0.58
16:P:19:ILE:HG22	16:P:36:ILE:CG1	2.32	0.58
1:A:394:G:H2'	1:A:395:C:H6	1.69	0.58
1:A:407:G:H2'	1:A:408:A:C8	2.38	0.58
1:A:421:U:O2'	1:A:422:C:H5'	2.03	0.58
1:A:532:A:N6	3:C:161:GLU:HB2	2.14	0.58
1:A:652:U:O4	1:A:752:G:O2'	2.14	0.58
1:A:1268:A:H2'	1:A:1269:A:C8	2.39	0.58
2:B:208:ILE:O	2:B:212:GLN:HB2	2.03	0.58
6:F:10:LEU:HD21	6:F:61:LEU:HD11	1.85	0.58
7:G:38:LEU:O	7:G:41:ARG:HB3	2.04	0.58
10:J:40:LEU:CD1	10:J:41:PRO:HD2	2.33	0.58
1:A:1069:C:O2'	1:A:1192:C:H1'	2.03	0.58
1:A:1330:U:OP1	13:M:23:TYR:O	2.20	0.58
1:A:1522:U:O2'	1:A:1523:G:H5'	2.03	0.58
3:C:130:VAL:HG11	3:C:157:ILE:CG2	2.32	0.58
9:I:111:ARG:HG2	9:I:112:LYS:N	2.18	0.58
10:J:3:LYS:HD3	10:J:76:ASN:N	2.16	0.58
22:X:2:G:H1	23:Y:36:C:N4	1.95	0.58
1:A:411:A:H1'	1:A:413:G:H1'	1.85	0.58
1:A:975:A:O2'	1:A:976:G:OP2	2.22	0.58
1:A:1096:C:H2'	1:A:1097:C:H6	1.68	0.58
1:A:1147:C:H4'	9:I:5:TYR:HE1	1.67	0.58
1:A:1225:A:H5'	1:A:1226:C:OP2	2.04	0.58
1:A:1406:U:H2'	1:A:1407:C:H5'	1.85	0.58
3:C:152:ILE:HG22	3:C:153:VAL:N	2.19	0.58
4:D:57:ARG:NE	4:D:205:GLU:OE2	2.36	0.58
4:D:150:GLU:HA	4:D:153:ARG:NE	2.19	0.58
7:G:57:GLU:HB3	7:G:58:PRO:HD2	1.84	0.58
14:N:9:LYS:HG3	14:N:21:TYR:O	2.02	0.58
20:T:74:LYS:HG3	20:T:75:ASN:N	2.18	0.58
1:A:513:C:H42	1:A:538:G:H1	1.52	0.58
4:D:58:LEU:HD22	4:D:62:GLN:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:177:ASP:OD1	4:D:179:GLU:HB2	2.03	0.58
10:J:6:ILE:HG22	10:J:98:ILE:HA	1.84	0.58
10:J:53:PRO:O	10:J:54:PHE:O	2.21	0.58
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.39	0.58
1:A:436:C:H5"	4:D:156:GLU:OE2	2.03	0.58
1:A:975:A:H4'	1:A:976:G:O5'	2.03	0.58
1:A:1123:A:H2	10:J:39:PRO:HG3	1.69	0.58
4:D:31:CYS:SG	4:D:32:ALA:N	2.77	0.58
4:D:108:LEU:HB3	4:D:110:PHE:CE1	2.39	0.58
5:E:129:ILE:H	5:E:129:ILE:CD1	2.13	0.58
16:P:67:THR:HG22	16:P:69:THR:H	1.68	0.58
19:S:23:ASN:C	19:S:25:LYS:H	2.05	0.58
1:A:445:G:H2'	1:A:446:G:H8	1.68	0.58
3:C:22:TRP:HA	10:J:93:GLY:HA3	1.84	0.58
4:D:120:LEU:O	4:D:126:ILE:HG12	2.03	0.58
9:I:8:GLY:HA2	9:I:79:LEU:CD1	2.29	0.58
12:L:60:LEU:HD21	12:L:66:VAL:CG2	2.27	0.58
1:A:514:C:H2'	1:A:515:G:H8	1.69	0.58
1:A:991:U:C4	1:A:1212:U:H1'	2.39	0.58
1:A:1255:G:H2'	1:A:1279:A:H62	1.68	0.58
2:B:8:LYS:HG3	2:B:48:MET:CE	2.34	0.58
2:B:28:PHE:CD2	2:B:190:THR:HA	2.39	0.58
2:B:185:ILE:HA	2:B:199:TYR:O	2.04	0.58
3:C:29:TYR:O	3:C:33:LEU:HB2	2.04	0.58
3:C:73:PRO:HA	3:C:76:VAL:CG2	2.34	0.58
7:G:89:MET:HA	7:G:155:ARG:NH2	2.19	0.58
8:H:120:THR:HG23	8:H:123:GLU:OE2	2.02	0.58
1:A:250:A:H2	1:A:274:A:N6	2.01	0.57
1:A:1221:G:H4'	19:S:53:ASN:O	2.04	0.57
2:B:42:ILE:HG22	2:B:43:ASP:N	2.18	0.57
1:A:523:A:N1	12:L:92:ASP:HB2	2.19	0.57
1:A:532:A:H2'	1:A:532:A:N3	2.17	0.57
1:A:1374:A:H2'	1:A:1375:A:H8	1.69	0.57
5:E:73:ASN:O	5:E:73:ASN:ND2	2.36	0.57
8:H:104:ARG:O	8:H:106:GLY:N	2.37	0.57
10:J:22:LYS:C	10:J:24:VAL:H	2.06	0.57
23:Y:34:C:H4'	23:Y:36:C:OP2	2.04	0.57
1:A:188:C:C2'	1:A:189:G:O2'	2.51	0.57
1:A:304:U:O2'	1:A:305:G:H5'	2.04	0.57
1:A:922:G:N3	1:A:1398:A:H2	2.02	0.57
1:A:1151:A:O2'	1:A:1152:A:H8	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:25:ARG:O	4:D:27:TYR:N	2.37	0.57
20:T:54:LYS:HG3	20:T:100:ILE:CD1	2.33	0.57
1:A:433:C:H2'	1:A:434:U:C6	2.39	0.57
1:A:434:U:H2'	1:A:435:C:H6	1.68	0.57
1:A:974:A:OP2	14:N:41:ARG:NH1	2.37	0.57
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.87	0.57
17:Q:59:ILE:CG2	17:Q:71:PHE:HB3	2.34	0.57
21:V:5:ASP:HB3	21:V:8:THR:OG1	2.05	0.57
1:A:390:C:O3'	16:P:28:ARG:NH2	2.37	0.57
4:D:78:LEU:HD13	4:D:97:LEU:HD23	1.86	0.57
7:G:32:ARG:O	7:G:34:GLY:N	2.38	0.57
13:M:79:LYS:HA	13:M:82:MET:HG3	1.87	0.57
20:T:33:ILE:CD1	20:T:63:ILE:HA	2.34	0.57
1:A:742:G:P	15:O:35:ARG:HH22	2.27	0.57
1:A:1321:C:O2'	19:S:77:THR:HG21	2.04	0.57
1:A:1427:U:H2'	1:A:1428:A:C8	2.39	0.57
2:B:18:GLY:H	2:B:42:ILE:H	1.52	0.57
3:C:19:GLU:O	3:C:56:ASP:HA	2.05	0.57
3:C:167:TRP:O	3:C:168:ALA:HB2	2.04	0.57
4:D:104:VAL:C	4:D:106:TYR:H	2.08	0.57
9:I:100:GLY:C	9:I:102:LEU:H	2.06	0.57
12:L:93:LEU:CD1	12:L:96:VAL:HG21	2.34	0.57
23:Y:39:A:H3'	23:Y:40:U:C6	2.39	0.57
1:A:9:G:OP1	5:E:122:GLU:HB2	2.05	0.57
1:A:191:G:C8	1:A:191:G:H3'	2.38	0.57
1:A:1006:A:OP2	1:A:1006(A):C:C5'	2.53	0.57
1:A:1182:G:O2'	1:A:1183:A:OP2	2.17	0.57
1:A:1299:A:C8	1:A:1301:U:H1'	2.40	0.57
3:C:39:ILE:C	3:C:41:GLY:H	2.07	0.57
6:F:68:PRO:HB2	6:F:71:ARG:CG	2.35	0.57
15:O:22:THR:O	15:O:27:VAL:HG11	2.04	0.57
1:A:1108:G:H4'	1:A:1191:A:O4'	2.04	0.57
1:A:1117:G:H21	1:A:1180:A:H1'	1.69	0.57
1:A:1365:G:O2'	1:A:1366:C:H5'	2.05	0.57
9:I:48:GLU:N	9:I:49:PRO:CD	2.68	0.57
10:J:49:VAL:HG11	14:N:41:ARG:O	2.05	0.57
18:R:28:GLU:OE1	18:R:28:GLU:N	2.38	0.57
1:A:191:G:C8	1:A:191:G:C3'	2.87	0.57
1:A:1037:C:H2'	1:A:1038:C:H6	1.70	0.57
1:A:1047:G:C2'	1:A:1048:G:H5'	2.34	0.57
1:A:1231:G:O3'	9:I:126:SER:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1406:U:O2'	1:A:1407:C:H5'	2.05	0.57
2:B:46:LYS:HA	2:B:49:GLU:OE1	2.05	0.57
4:D:23:GLY:HA3	4:D:112:VAL:HB	1.86	0.57
5:E:148:VAL:HG21	8:H:107:LEU:HD13	1.87	0.57
8:H:23:SER:HA	8:H:63:LEU:CD2	2.34	0.57
9:I:8:GLY:CA	9:I:79:LEU:HD12	2.31	0.57
14:N:26:ARG:CD	14:N:47:LEU:HD11	2.35	0.57
1:A:188:C:N3	1:A:189:G:N3	2.53	0.57
1:A:429:U:H6	4:D:25:ARG:HH22	1.52	0.57
1:A:1115:C:H2'	1:A:1116:C:H6	1.70	0.57
3:C:177:THR:HG23	3:C:177:THR:O	2.05	0.57
8:H:41:ARG:HG2	8:H:41:ARG:HH11	1.70	0.57
9:I:102:LEU:HD23	9:I:102:LEU:N	2.18	0.57
13:M:78:ILE:C	13:M:80:ARG:N	2.58	0.57
1:A:952:U:H2'	1:A:953:G:H8	1.70	0.56
1:A:994:A:N7	1:A:1216:G:H4'	2.20	0.56
3:C:28:GLN:HA	3:C:31:HIS:HD2	1.70	0.56
5:E:144:THR:O	5:E:148:VAL:HG23	2.04	0.56
7:G:138:LYS:C	7:G:140:ASP:H	2.07	0.56
7:G:156:TRP:HA	7:G:156:TRP:CE3	2.40	0.56
20:T:29:LYS:O	20:T:32:ALA:HB3	2.04	0.56
1:A:50:A:N6	1:A:361:G:H4'	2.20	0.56
1:A:191:G:H22	20:T:85:MET:HE1	1.70	0.56
1:A:530:G:O6	22:X:3:G:C1'	2.43	0.56
1:A:1016:A:H2'	1:A:1017:G:O4'	2.05	0.56
1:A:1256:A:H4'	1:A:1257:U:H5'	1.87	0.56
1:A:1515:C:O2'	1:A:1516:G:H5'	2.05	0.56
10:J:45:ARG:O	10:J:46:ARG:HG2	2.05	0.56
11:K:48:ILE:CG2	11:K:49:GLY:H	2.04	0.56
12:L:36:VAL:O	12:L:81:SER:O	2.22	0.56
1:A:319:G:O2'	1:A:320:C:H5'	2.05	0.56
1:A:972:C:C4'	10:J:57:LYS:HG2	2.26	0.56
1:A:976:G:N7	1:A:1358:U:C2	2.73	0.56
1:A:976:G:C8	1:A:1358:U:O2	2.57	0.56
1:A:1072:G:H1	1:A:1103:C:H42	1.52	0.56
1:A:1150:U:O2	10:J:39:PRO:HG2	2.05	0.56
1:A:1273:G:H2'	1:A:1274:G:C8	2.40	0.56
1:A:1327:C:OP2	21:V:12:LYS:NZ	2.38	0.56
1:A:1476:G:O2'	1:A:1477:C:H5'	2.05	0.56
3:C:71:ALA:CB	3:C:109:PRO:HB3	2.36	0.56
3:C:178:LEU:O	3:C:179:ARG:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:THR:HG21	3:C:193:TYR:CZ	2.40	0.56
4:D:3:ARG:NE	4:D:118:ARG:NH1	2.53	0.56
4:D:126:ILE:CG2	4:D:127:THR:N	2.69	0.56
4:D:162:LEU:CD1	4:D:181:MET:HG2	2.34	0.56
5:E:31:LEU:HD13	5:E:43:LEU:HD21	1.85	0.56
5:E:80:ILE:HG13	5:E:91:LEU:HB2	1.87	0.56
7:G:77:SER:O	7:G:78:ARG:HB2	2.04	0.56
8:H:104:ARG:O	8:H:107:LEU:N	2.38	0.56
9:I:15:ALA:HB2	9:I:65:VAL:HG23	1.86	0.56
17:Q:67:LYS:O	17:Q:68:ARG:HB3	2.05	0.56
20:T:10:LEU:C	20:T:12:ALA:H	2.09	0.56
1:A:265:G:H2'	1:A:267:C:C5	2.35	0.56
1:A:738:C:P	6:F:92:LYS:HD3	2.45	0.56
1:A:1197:G:H2'	1:A:1198:G:H5'	1.87	0.56
8:H:68:ARG:HG2	8:H:68:ARG:NH1	2.20	0.56
8:H:108:GLY:HA3	8:H:138:TRP:HB3	1.87	0.56
15:O:3:ILE:HG13	15:O:38:ARG:NH1	2.20	0.56
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.88	0.56
18:R:21:LYS:O	18:R:23:LYS:N	2.38	0.56
1:A:188:C:H2'	1:A:189:G:C2'	2.35	0.56
1:A:601:C:O2'	1:A:602:A:H5'	2.06	0.56
1:A:948:C:O2'	1:A:949:A:H5'	2.05	0.56
1:A:1124:G:H5'	10:J:35:SER:O	2.05	0.56
1:A:1162:C:O2'	1:A:1163:C:H5'	2.06	0.56
1:A:1494:G:O2'	1:A:1495:U:H5'	2.05	0.56
2:B:110:GLN:HA	2:B:113:HIS:HB2	1.86	0.56
8:H:17:THR:O	8:H:78:GLN:NE2	2.38	0.56
11:K:100:ALA:O	11:K:102:GLY:N	2.38	0.56
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.40	0.56
17:Q:68:ARG:HG2	17:Q:68:ARG:HH11	1.70	0.56
18:R:39:VAL:O	18:R:42:ARG:HB2	2.05	0.56
1:A:103:C:P	20:T:17:ARG:NH1	2.79	0.56
1:A:148:G:H2'	1:A:149:A:H8	1.70	0.56
1:A:718:G:H4'	11:K:117:ASN:HD22	1.71	0.56
1:A:1500:A:O2'	1:A:1501:C:H5'	2.06	0.56
2:B:68:ILE:HB	2:B:90:MET:HE3	1.88	0.56
3:C:131:ARG:HD3	5:E:50:GLU:OE2	2.05	0.56
10:J:42:THR:HG23	10:J:67:THR:C	2.26	0.56
12:L:119:LYS:O	12:L:120:TYR:HB2	2.05	0.56
19:S:15:LEU:HD22	19:S:49:ILE:HD13	1.86	0.56
1:A:322:C:O2'	1:A:323:U:H5'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:C:H1'	14:N:4:LYS:CE	2.35	0.56
1:A:1539:C:H42	7:G:82:GLY:HA2	1.71	0.56
3:C:175:LEU:HD23	3:C:182:ILE:HD13	1.87	0.56
9:I:106:ALA:O	9:I:108:VAL:HG23	2.05	0.56
1:A:189:G:C2	1:A:190:C:C1'	2.81	0.56
1:A:279:A:OP2	17:Q:95:TYR:OH	2.20	0.56
1:A:1228:C:H4'	13:M:116:THR:HA	1.87	0.56
1:A:1251:A:H4'	9:I:12:GLU:OE2	2.06	0.56
3:C:120:VAL:O	3:C:124:ILE:HG13	2.06	0.56
3:C:131:ARG:HH21	3:C:164:ARG:NH2	2.04	0.56
3:C:155:GLY:O	3:C:157:ILE:N	2.39	0.56
5:E:79:GLU:OE2	8:H:105:ARG:HG2	2.06	0.56
5:E:83:GLU:HG2	5:E:88:LYS:HG3	1.88	0.56
18:R:58:LEU:HD11	18:R:66:LEU:HD22	1.86	0.56
1:A:1061:G:O4'	10:J:56:HIS:CD2	2.59	0.56
1:A:1347:G:O2'	1:A:1348:U:P	2.63	0.56
3:C:90:GLU:HA	3:C:93:LYS:CG	2.35	0.56
9:I:118:LYS:NZ	9:I:118:LYS:CB	2.69	0.56
11:K:29:ILE:C	11:K:29:ILE:HD12	2.26	0.56
15:O:39:LEU:O	15:O:39:LEU:HD13	2.05	0.56
1:A:191:G:H8	1:A:191:G:H3'	1.70	0.56
1:A:202:U:H5"	1:A:203:U:OP2	2.06	0.56
1:A:344:A:H4'	1:A:345:C:OP2	2.06	0.56
1:A:922:G:H2'	1:A:923:A:C8	2.40	0.56
3:C:139:GLN:O	3:C:143:GLU:N	2.38	0.56
3:C:201:TYR:C	3:C:202:ILE:HG13	2.26	0.56
9:I:64:THR:HG22	9:I:66:ARG:HH12	1.71	0.56
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.88	0.56
13:M:25:ILE:HD11	13:M:60:VAL:CG1	2.36	0.56
13:M:98:VAL:O	13:M:98:VAL:HG12	2.04	0.56
1:A:1197:G:OP2	1:A:1198:G:OP2	2.23	0.55
9:I:26:VAL:HG13	9:I:61:ALA:CB	2.36	0.55
19:S:30:LEU:O	19:S:31:ILE:HD13	2.06	0.55
1:A:456:C:H2'	1:A:457:C:C6	2.42	0.55
1:A:613:C:O2'	1:A:614:A:H5'	2.06	0.55
1:A:1318:A:H4'	19:S:10:PHE:CD2	2.42	0.55
1:A:1321:C:H5"	13:M:87:TYR:CE2	2.40	0.55
1:A:1366:C:C6	1:A:1367:C:H5	2.23	0.55
1:A:1368:G:O2'	1:A:1369:C:H5'	2.06	0.55
1:A:1372:U:C2'	1:A:1373:G:H5'	2.36	0.55
1:A:1512:U:O2'	1:A:1513:A:H5'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:GLY:C	2:B:108:ILE:HD12	2.26	0.55
3:C:66:VAL:HG12	3:C:67:THR:N	2.20	0.55
7:G:143:ARG:O	7:G:147:ALA:HB2	2.05	0.55
8:H:14:ARG:CB	8:H:14:ARG:NH1	2.68	0.55
8:H:20:TYR:CZ	8:H:75:ARG:HB3	2.41	0.55
12:L:40:VAL:O	12:L:40:VAL:HG12	2.05	0.55
1:A:412:A:C2	4:D:35:ARG:CG	2.87	0.55
1:A:792:A:H1'	1:A:794:A:N7	2.21	0.55
1:A:1397:C:N4	22:X:4:G:H2'	2.22	0.55
5:E:137:GLU:O	5:E:141:GLN:HB2	2.07	0.55
7:G:6:ARG:HG2	7:G:6:ARG:O	2.05	0.55
7:G:59:LEU:O	7:G:61:VAL:N	2.38	0.55
7:G:136:LYS:C	7:G:138:LYS:H	2.08	0.55
13:M:29:ARG:HB3	13:M:64:TRP:CH2	2.41	0.55
13:M:74:VAL:HA	13:M:77:ASN:HB3	1.89	0.55
14:N:27:CYS:SG	14:N:29:ARG:CG	2.94	0.55
16:P:28:ARG:HH11	16:P:28:ARG:HG3	1.71	0.55
1:A:308:C:H2'	1:A:309:G:H8	1.71	0.55
1:A:353:A:H5'	1:A:353:A:H8	1.71	0.55
1:A:840:C:H4'	1:A:848:C:C2	2.40	0.55
1:A:1124:G:HO2'	1:A:1145:C:H41	1.54	0.55
1:A:1132:C:H2'	1:A:1133:G:C8	2.42	0.55
1:A:1305:G:O2'	1:A:1331:G:N2	2.39	0.55
1:A:1497:G:H2'	1:A:1498:U:H5'	1.88	0.55
2:B:212:GLN:NE2	2:B:235:SER:HB2	2.22	0.55
5:E:11:ILE:CG2	5:E:105:VAL:HG22	2.36	0.55
13:M:31:LYS:O	13:M:35:GLU:HB2	2.06	0.55
18:R:29:PHE:CE1	18:R:31:LEU:HD23	2.41	0.55
1:A:1094:G:O5'	1:A:1095:U:H5	1.89	0.55
2:B:157:ARG:O	2:B:158:LEU:C	2.45	0.55
3:C:52:LEU:HD12	3:C:52:LEU:O	2.07	0.55
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.87	0.55
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.89	0.55
5:E:9:LYS:HD3	5:E:112:LEU:CD2	2.36	0.55
8:H:112:LEU:HD23	8:H:112:LEU:N	2.22	0.55
9:I:65:VAL:HG21	9:I:73:GLN:HB3	1.87	0.55
18:R:53:ARG:C	18:R:55:ARG:H	2.10	0.55
1:A:687:A:H4'	1:A:688:G:O5'	2.06	0.55
1:A:748:C:H1'	1:A:749:C:H5	1.72	0.55
2:B:55:PHE:O	2:B:58:ILE:HB	2.06	0.55
10:J:49:VAL:HG13	14:N:41:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:9:LYS:HD3	14:N:9:LYS:C	2.27	0.55
23:Y:35:C:H2'	23:Y:36:C:H6	1.72	0.55
1:A:36:C:O2'	1:A:37:U:H5'	2.06	0.55
1:A:968:A:H4'	1:A:969:A:OP2	2.07	0.55
1:A:1149:C:H2'	1:A:1150:U:C6	2.41	0.55
1:A:1347:G:C6	9:I:107:ARG:NH1	2.75	0.55
1:A:1369:C:H2'	1:A:1370:G:H8	1.66	0.55
1:A:1490:C:H6	1:A:1490:C:C5'	2.10	0.55
3:C:113:ALA:HB3	3:C:114:PRO:HD3	1.89	0.55
4:D:13:ARG:HD2	4:D:38:TYR:O	2.07	0.55
6:F:69:GLU:O	6:F:71:ARG:N	2.39	0.55
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.89	0.55
1:A:29:G:O2'	1:A:30:U:H5'	2.07	0.55
1:A:116:A:H61	1:A:313:A:H1'	1.72	0.55
1:A:359:U:O2'	1:A:360:A:H5'	2.07	0.55
1:A:432:A:H2'	1:A:433:C:O4'	2.06	0.55
1:A:533:A:C5	1:A:536:C:C4	2.95	0.55
1:A:991:U:O2'	1:A:993:G:H8	1.90	0.55
1:A:1410:G:C4	1:A:1491:G:N2	2.74	0.55
2:B:69:LEU:C	2:B:69:LEU:CD2	2.75	0.55
5:E:90:VAL:O	5:E:120:THR:HA	2.06	0.55
6:F:37:VAL:HG12	6:F:38:GLU:N	2.21	0.55
8:H:100:ILE:HD13	8:H:112:LEU:HD11	1.87	0.55
10:J:4:ILE:HB	10:J:74:ILE:H	1.72	0.55
1:A:457:C:H2'	1:A:458:C:H5	1.72	0.55
1:A:639:G:O2'	1:A:640:A:H5'	2.07	0.55
2:B:13:ALA:HB1	2:B:17:PHE:HE2	1.71	0.55
3:C:137:ALA:HA	3:C:140:ARG:HH11	1.72	0.55
6:F:94:GLN:HE21	18:R:32:ARG:HD3	1.70	0.55
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.22	0.55
1:A:407:G:H2'	1:A:408:A:H8	1.71	0.55
1:A:651:C:O2'	1:A:652:U:H5'	2.07	0.55
1:A:1443:G:H4'	1:A:1446:A:C5'	2.35	0.55
1:A:1508:G:O2'	1:A:1509:C:H5'	2.07	0.55
2:B:240:GLN:CD	2:B:240:GLN:H	2.10	0.55
3:C:179:ARG:HD3	3:C:207:VAL:N	2.21	0.55
10:J:35:SER:HB2	10:J:72:VAL:O	2.07	0.55
14:N:29:ARG:O	14:N:30:ALA:HB2	2.08	0.55
15:O:65:ARG:HH11	15:O:65:ARG:CB	2.14	0.55
18:R:58:LEU:CD1	18:R:66:LEU:HD22	2.36	0.55
1:A:21:G:H2'	1:A:22:G:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:A:H2'	1:A:357:G:H8	1.72	0.54
1:A:1002:G:H2'	1:A:1003:G:C8	2.42	0.54
1:A:1005:A:H1'	1:A:1036:G:H22	1.72	0.54
1:A:1052:U:H5"	23:Y:34:C:C6	2.42	0.54
1:A:1104:G:OP1	2:B:111:ARG:HD2	2.07	0.54
1:A:1200:C:H1'	1:A:1204:A:H61	1.71	0.54
1:A:1286:A:C2	21:V:18:TYR:OH	2.60	0.54
1:A:1347:G:C5	9:I:107:ARG:NH1	2.75	0.54
3:C:95:THR:HB	3:C:97:LYS:HE2	1.87	0.54
8:H:6:ILE:HD11	8:H:31:PHE:CD2	2.42	0.54
15:O:74:ASP:HB3	15:O:77:ARG:HB2	1.88	0.54
17:Q:65:ILE:HD12	17:Q:65:ILE:N	2.23	0.54
1:A:36:C:H2'	1:A:37:U:H5'	1.88	0.54
1:A:254:G:O2'	1:A:255:G:H5'	2.07	0.54
1:A:1249:C:O4'	9:I:70:LYS:HD3	2.07	0.54
5:E:43:LEU:HD22	5:E:44:GLY:N	2.22	0.54
12:L:42:THR:HG21	12:L:52:LEU:HD22	1.89	0.54
1:A:383:A:C2'	1:A:384:G:H5'	2.34	0.54
1:A:424:G:O2'	1:A:425:G:H5'	2.07	0.54
1:A:1124:G:HO2'	1:A:1145:C:N4	2.05	0.54
1:A:1339:A:H2'	1:A:1340:A:O4'	2.08	0.54
2:B:58:ILE:HG23	2:B:68:ILE:HD11	1.89	0.54
2:B:107:THR:C	2:B:109:SER:H	2.10	0.54
2:B:215:LEU:HD23	2:B:215:LEU:O	2.08	0.54
7:G:3:ARG:HG2	7:G:3:ARG:NH1	2.22	0.54
7:G:156:TRP:HA	7:G:156:TRP:HE3	1.72	0.54
11:K:46:GLY:O	11:K:48:ILE:O	2.26	0.54
11:K:84:VAL:HG12	11:K:85:ARG:N	2.22	0.54
17:Q:76:LEU:HD23	17:Q:76:LEU:C	2.27	0.54
17:Q:104:LYS:HD3	17:Q:105:ALA:N	2.23	0.54
1:A:389:A:H2'	1:A:390:C:H5'	1.90	0.54
1:A:501:C:O2'	1:A:502:G:H5'	2.07	0.54
1:A:853:G:O2'	1:A:854:G:H5'	2.07	0.54
1:A:1072:G:H2'	1:A:1073:U:H6	1.73	0.54
1:A:1381:U:O2'	1:A:1382:C:H5'	2.08	0.54
4:D:34:GLU:O	4:D:35:ARG:HB3	2.07	0.54
10:J:46:ARG:HG2	10:J:46:ARG:HH11	1.72	0.54
12:L:92:ASP:HB3	12:L:93:LEU:HD23	1.88	0.54
14:N:45:ARG:HG3	14:N:45:ARG:NH1	2.21	0.54
17:Q:63:ARG:O	17:Q:65:ILE:CD1	2.54	0.54
1:A:408:A:O2'	1:A:409:G:H5'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:A:H2'	1:A:947:G:H8	1.71	0.54
1:A:1014:A:H2'	1:A:1015:A:C8	2.43	0.54
1:A:1477:C:H2'	1:A:1478:C:C6	2.40	0.54
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.43	0.54
8:H:103:VAL:HG12	8:H:108:GLY:HA3	1.90	0.54
9:I:43:ALA:HA	9:I:74:ILE:HG23	1.88	0.54
10:J:77:PRO:CA	10:J:82:ILE:HD11	2.37	0.54
18:R:86:VAL:HG12	18:R:87:ARG:H	1.72	0.54
1:A:106:C:O2'	1:A:107:G:H5'	2.08	0.54
1:A:145:G:O2'	1:A:146:G:H5'	2.07	0.54
1:A:328:C:O2	1:A:328:C:C2'	2.56	0.54
1:A:556:C:O2'	1:A:557:G:H5'	2.08	0.54
1:A:1053:G:H4'	1:A:1054:C:H3'	1.89	0.54
2:B:151:GLY:O	2:B:153:ARG:N	2.40	0.54
12:L:32:PHE:HA	12:L:85:ILE:O	2.08	0.54
12:L:46:LYS:HG2	12:L:47:LYS:HG3	1.89	0.54
18:R:26:LEU:HD23	18:R:29:PHE:CE2	2.42	0.54
1:A:62:U:H2'	1:A:63:C:H5"	1.88	0.54
1:A:383:A:H2'	1:A:384:G:C5'	2.36	0.54
1:A:760:G:H2'	1:A:761:G:H5'	1.88	0.54
1:A:947:G:H2'	1:A:948:C:C6	2.43	0.54
1:A:1241:G:H2'	1:A:1242:C:H6	1.71	0.54
1:A:1327:C:H5"	21:V:20:LYS:HB3	1.87	0.54
2:B:208:ILE:HA	2:B:211:ILE:HD12	1.88	0.54
3:C:6:HIS:HD2	3:C:9:GLY:N	2.03	0.54
6:F:14:LEU:CD2	6:F:18:GLN:HB2	2.37	0.54
7:G:15:ASP:OD1	7:G:18:TYR:HB2	2.08	0.54
7:G:17:VAL:HG12	7:G:18:TYR:N	2.21	0.54
7:G:47:CYS:HA	7:G:50:ILE:HD12	1.90	0.54
12:L:53:ARG:NH1	12:L:92:ASP:OD2	2.41	0.54
12:L:126:LYS:HD2	12:L:126:LYS:O	2.07	0.54
1:A:189:G:C4	1:A:190:C:C6	2.95	0.54
1:A:1276:G:O2'	1:A:1277:C:H5'	2.07	0.54
1:A:1286:A:H2	21:V:18:TYR:OH	1.91	0.54
5:E:10:MET:HA	5:E:32:VAL:HG23	1.90	0.54
5:E:101:ILE:HD12	5:E:119:LEU:CD2	2.37	0.54
7:G:121:ALA:O	7:G:125:MET:HG3	2.07	0.54
9:I:105:ASP:OD1	9:I:107:ARG:HB2	2.07	0.54
10:J:23:ILE:O	10:J:23:ILE:HG22	2.07	0.54
20:T:10:LEU:O	20:T:10:LEU:HD13	2.08	0.54
20:T:67:ALA:O	20:T:73:HIS:CD2	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:G:H5"	3:C:154:SER:HB2	1.90	0.54
1:A:1481:U:O2'	1:A:1482:G:H5'	2.08	0.54
2:B:43:ASP:OD1	2:B:45:GLN:HB2	2.08	0.54
3:C:11:ARG:HG3	3:C:178:LEU:HD12	1.90	0.54
3:C:140:ARG:HG3	3:C:141:VAL:N	2.23	0.54
9:I:4:TYR:CZ	9:I:88:TYR:HD1	2.26	0.54
13:M:69:GLU:O	13:M:73:GLU:HB2	2.08	0.54
16:P:70:ALA:O	16:P:74:LEU:HB2	2.07	0.54
1:A:105:G:H2'	1:A:106:C:C6	2.42	0.54
1:A:1037:C:H2'	1:A:1038:C:C6	2.43	0.54
1:A:1058:G:OP1	3:C:199:LYS:HE3	2.07	0.54
3:C:178:LEU:O	3:C:179:ARG:CB	2.56	0.54
8:H:85:ARG:HD3	8:H:86:ILE:N	2.23	0.54
9:I:58:ARG:HB2	9:I:58:ARG:CZ	2.37	0.54
13:M:27:LYS:O	13:M:30:ALA:HB3	2.08	0.54
15:O:78:TYR:CE1	15:O:82:ILE:HD11	2.43	0.54
1:A:543:C:O2'	1:A:544:G:H5'	2.08	0.53
1:A:877:C:O2'	1:A:878:G:H5'	2.07	0.53
1:A:954:G:N2	1:A:1227:A:H62	1.99	0.53
1:A:1249:C:O2'	1:A:1250:A:H5'	2.07	0.53
4:D:7:PRO:HG2	4:D:10:ARG:HD2	1.89	0.53
5:E:80:ILE:CD1	5:E:138:ALA:HB1	2.28	0.53
7:G:16:LEU:HD22	7:G:16:LEU:N	2.21	0.53
8:H:13:ILE:O	8:H:17:THR:HG23	2.07	0.53
9:I:5:TYR:CD2	9:I:6:GLY:N	2.74	0.53
12:L:93:LEU:O	12:L:96:VAL:HG23	2.08	0.53
13:M:29:ARG:HA	13:M:32:GLU:HB3	1.89	0.53
16:P:51:VAL:O	16:P:52:ASP:CB	2.45	0.53
19:S:20:LEU:HA	19:S:23:ASN:ND2	2.22	0.53
1:A:349:A:C3'	1:A:350:G:H5"	2.38	0.53
1:A:1003:G:H3'	1:A:1004:A:H5"	1.90	0.53
1:A:1060:C:H2'	1:A:1061:G:C8	2.39	0.53
1:A:1256:A:H5'	1:A:1258:G:H1'	1.90	0.53
1:A:1360:A:H2'	1:A:1361:G:C8	2.42	0.53
1:A:1497:G:O2'	1:A:1498:U:H5'	2.07	0.53
2:B:97:TRP:CH2	2:B:176:GLU:OE2	2.61	0.53
2:B:167:PRO:HG3	2:B:188:ALA:HB2	1.88	0.53
3:C:72:LYS:C	3:C:74:GLY:H	2.11	0.53
3:C:74:GLY:O	3:C:76:VAL:N	2.41	0.53
3:C:137:ALA:HA	3:C:140:ARG:NH1	2.22	0.53
7:G:133:GLY:O	7:G:136:LYS:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:5:ARG:HD2	10:J:99:LYS:HB2	1.90	0.53
12:L:27:LEU:O	12:L:28:LYS:HB3	2.08	0.53
16:P:1:MET:HE1	16:P:3:LYS:HE3	1.90	0.53
17:Q:74:LEU:O	17:Q:75:ARG:HB3	2.08	0.53
19:S:12:ASP:OD1	19:S:37:ARG:HD2	2.08	0.53
1:A:342:C:H42	1:A:347:G:H1	1.55	0.53
1:A:1015:A:H2'	1:A:1016:A:H8	1.71	0.53
7:G:15:ASP:HB3	7:G:19:GLY:CA	2.38	0.53
7:G:46:ALA:O	7:G:50:ILE:HG13	2.08	0.53
20:T:51:GLU:O	20:T:55:ILE:HG13	2.09	0.53
1:A:344:A:H5"	1:A:345:C:H5	1.73	0.53
1:A:791:G:H2'	1:A:792:A:C5'	2.38	0.53
1:A:791:G:C2'	1:A:792:A:H5'	2.37	0.53
2:B:114:ARG:C	2:B:116:GLU:H	2.12	0.53
3:C:31:HIS:C	3:C:33:LEU:H	2.12	0.53
4:D:151:LYS:H	4:D:151:LYS:HD2	1.74	0.53
5:E:51:VAL:O	5:E:55:VAL:HG23	2.08	0.53
8:H:30:ARG:HB3	8:H:30:ARG:NH1	2.23	0.53
10:J:7:LYS:NZ	10:J:99:LYS:NZ	2.56	0.53
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.90	0.53
20:T:13:LEU:H	20:T:13:LEU:HD12	1.72	0.53
1:A:474:G:C5'	1:A:475:G:N7	2.69	0.53
1:A:590:C:O2'	1:A:591:U:H5'	2.08	0.53
1:A:792:A:H4'	1:A:793:U:C5'	2.38	0.53
2:B:80:ILE:CD1	2:B:208:ILE:HG23	2.26	0.53
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.90	0.53
3:C:70:VAL:N	3:C:106:VAL:HG23	2.23	0.53
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.89	0.53
4:D:114:ARG:HG3	4:D:114:ARG:NH1	2.23	0.53
7:G:41:ARG:HG2	7:G:42:ILE:N	2.23	0.53
1:A:263:A:P	20:T:79:ARG:HH12	2.32	0.53
1:A:742:G:OP2	15:O:35:ARG:NH2	2.41	0.53
1:A:865:A:H2'	1:A:866:C:C6	2.43	0.53
1:A:938:A:N6	1:A:939:G:C6	2.76	0.53
1:A:1196:U:OP1	1:A:1197:G:H5"	2.09	0.53
4:D:80:GLU:O	4:D:84:LYS:HG3	2.08	0.53
7:G:18:TYR:OH	7:G:58:PRO:HB2	2.08	0.53
13:M:11:ARG:CZ	13:M:12:ASN:H	2.20	0.53
20:T:13:LEU:HD12	20:T:13:LEU:N	2.24	0.53
1:A:93:G:H2'	1:A:93:G:N3	2.23	0.53
1:A:620:C:C1'	4:D:135:LEU:HD13	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1249:C:H2'	1:A:1250:A:H5'	1.90	0.53
1:A:1262:C:O2'	1:A:1263:C:H5'	2.08	0.53
3:C:58:GLU:HG3	10:J:92:THR:HG21	1.89	0.53
4:D:25:ARG:C	4:D:27:TYR:N	2.61	0.53
11:K:90:GLY:O	11:K:91:ARG:C	2.46	0.53
14:N:42:ILE:O	14:N:45:ARG:HB3	2.07	0.53
16:P:26:ARG:HH11	16:P:26:ARG:CB	2.21	0.53
1:A:384:G:H2'	1:A:385:C:H6	1.73	0.53
1:A:551:U:H2'	1:A:552:U:C6	2.44	0.53
1:A:950:U:O4	13:M:105:THR:HG21	2.08	0.53
1:A:1166:G:H2'	1:A:1166:G:N3	2.22	0.53
1:A:1345:U:C4	1:A:1377:A:C2	2.97	0.53
9:I:16:ARG:HB2	9:I:64:THR:HB	1.89	0.53
11:K:48:ILE:HD13	11:K:63:LEU:HB3	1.90	0.53
11:K:59:TYR:CZ	11:K:63:LEU:HD21	2.44	0.53
1:A:405:U:O4	4:D:2:GLY:N	2.42	0.53
1:A:581:G:O6	1:A:758:G:H3'	2.08	0.53
1:A:674:G:H2'	1:A:675:A:C8	2.43	0.53
4:D:141:ARG:HB3	4:D:142:PRO:HD2	1.91	0.53
5:E:11:ILE:HD11	5:E:33:VAL:HG23	1.89	0.53
7:G:89:MET:HA	7:G:155:ARG:NH1	2.23	0.53
16:P:67:THR:HG22	16:P:69:THR:N	2.24	0.53
1:A:540:G:H2'	1:A:541:G:O4'	2.08	0.53
1:A:1027:C:O2'	1:A:1028:C:H5'	2.09	0.53
1:A:1239:A:H62	1:A:1299:A:H62	1.57	0.53
1:A:1281:U:H4'	1:A:1282:C:OP2	2.09	0.53
1:A:1466:C:H2'	1:A:1467:G:O4'	2.09	0.53
3:C:136:GLN:O	3:C:139:GLN:HB2	2.08	0.53
5:E:15:ARG:HD3	5:E:26:PHE:CD2	2.44	0.53
6:F:10:LEU:HD11	6:F:59:TYR:HD2	1.74	0.53
19:S:15:LEU:HD23	19:S:33:THR:OG1	2.09	0.53
1:A:21:G:C2	1:A:22:G:C5	2.98	0.52
1:A:141:A:H1'	1:A:182:U:O2	2.09	0.52
1:A:356:A:H1'	1:A:368:U:O2'	2.10	0.52
1:A:357:G:H1'	1:A:368:U:O2	2.08	0.52
1:A:501:C:H2'	1:A:502:G:C8	2.29	0.52
1:A:736:C:O3'	6:F:91:VAL:HG23	2.09	0.52
1:A:1004:A:N7	1:A:1026:G:N7	2.57	0.52
1:A:1006(A):C:H3'	1:A:1007:C:C6	2.43	0.52
1:A:1498:U:C4'	1:A:1519:A:H2	2.17	0.52
4:D:162:LEU:O	4:D:162:LEU:HD23	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:C:H2'	1:A:268:C:C6	2.44	0.52
1:A:457:C:H2'	1:A:458:C:C5	2.45	0.52
1:A:689:C:P	11:K:46:GLY:HA3	2.49	0.52
3:C:64:VAL:HG12	3:C:65:ALA:N	2.23	0.52
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.09	0.52
5:E:110:LEU:O	5:E:113:ALA:HB3	2.09	0.52
5:E:116:THR:HG23	5:E:117:ASP:N	2.25	0.52
11:K:69:ALA:O	11:K:72:ALA:HB3	2.09	0.52
11:K:84:VAL:HG21	11:K:95:ILE:HD11	1.92	0.52
13:M:36:LYS:HG3	13:M:59:TYR:OH	2.09	0.52
19:S:30:LEU:HD13	19:S:30:LEU:C	2.29	0.52
19:S:45:VAL:HG12	19:S:46:GLY:N	2.23	0.52
20:T:33:ILE:HD11	20:T:63:ILE:HA	1.90	0.52
1:A:244:U:O4	1:A:906:G:H1'	2.09	0.52
1:A:333:G:H4'	20:T:16:HIS:NE2	2.24	0.52
1:A:1086:U:H3	1:A:1099:G:N2	2.05	0.52
1:A:1130:A:H4'	9:I:20:ARG:NH2	2.25	0.52
1:A:1213:A:N1	1:A:1215:G:H1'	2.25	0.52
5:E:62:ALA:O	5:E:64:ARG:O	2.27	0.52
6:F:65:VAL:HG23	6:F:66:GLU:N	2.24	0.52
1:A:33:A:H2'	1:A:34:C:H6	1.74	0.52
1:A:282:A:C2	1:A:283:C:H1'	2.45	0.52
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.42	0.52
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.43	0.52
5:E:28:PHE:HD1	5:E:49:PRO:O	1.92	0.52
5:E:76:ILE:HG23	5:E:142:LEU:CD1	2.39	0.52
9:I:70:LYS:O	9:I:74:ILE:HG13	2.09	0.52
12:L:55:VAL:O	12:L:70:ILE:HD11	2.10	0.52
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.91	0.52
1:A:112:G:H4'	1:A:389:A:H5"	1.90	0.52
1:A:296:U:H2'	1:A:297:G:C8	2.44	0.52
1:A:695:A:H2'	1:A:696:A:O4'	2.08	0.52
1:A:1207:G:H2'	1:A:1208:C:C6	2.44	0.52
6:F:19:LEU:O	6:F:23:LYS:HG3	2.09	0.52
11:K:111:ASP:CG	11:K:111:ASP:O	2.45	0.52
12:L:98:TYR:N	12:L:98:TYR:CD1	2.77	0.52
16:P:19:ILE:CG2	16:P:36:ILE:HG13	2.38	0.52
17:Q:93:GLN:OE1	17:Q:93:GLN:HA	2.09	0.52
1:A:428:G:O4'	1:A:430:A:C8	2.63	0.52
1:A:991:U:O2'	1:A:993:G:C8	2.63	0.52
1:A:1161:C:H2'	1:A:1162:C:H6	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1256:A:H5'	1:A:1258:G:C1'	2.39	0.52
1:A:1273:G:H2'	1:A:1274:G:H8	1.73	0.52
1:A:1320:C:C2	19:S:72:GLY:HA3	2.45	0.52
1:A:1347:G:C8	9:I:107:ARG:HB3	2.44	0.52
3:C:10:PHE:CZ	3:C:178:LEU:HD22	2.45	0.52
9:I:26:VAL:HA	9:I:61:ALA:HB3	1.92	0.52
11:K:14:VAL:HG13	11:K:35:PRO:HD3	1.91	0.52
11:K:34:ASP:HB2	11:K:35:PRO:CD	2.39	0.52
17:Q:80:GLY:O	17:Q:81:ARG:CB	2.58	0.52
20:T:84:LEU:C	20:T:86:ARG:H	2.13	0.52
1:A:166:G:O2'	1:A:167:G:H5'	2.10	0.52
1:A:333:G:H4'	20:T:16:HIS:CD2	2.45	0.52
1:A:570:G:H2'	1:A:571:U:C6	2.45	0.52
1:A:1526:G:H2'	1:A:1527:C:C6	2.45	0.52
3:C:156:ARG:HB3	3:C:160:ALA:O	2.09	0.52
9:I:16:ARG:O	9:I:63:ILE:HG23	2.10	0.52
1:A:337:C:H2'	1:A:338:A:C8	2.45	0.52
1:A:349:A:C2'	1:A:350:G:H5"	2.40	0.52
1:A:406:G:H5"	4:D:5:ILE:CG2	2.39	0.52
1:A:449:C:H2'	1:A:450:G:O4'	2.10	0.52
1:A:1108:G:H5'	1:A:1191:A:H4'	1.91	0.52
1:A:1298:C:H2'	7:G:114:ARG:HH12	1.75	0.52
1:A:1298:C:H2'	7:G:114:ARG:NH1	2.24	0.52
1:A:1367:C:H4'	10:J:48:THR:HG21	1.92	0.52
1:A:1492:A:O2'	1:A:1493:A:C8	2.60	0.52
3:C:47:LEU:HD23	3:C:68:VAL:HG11	1.90	0.52
4:D:150:GLU:HB3	4:D:153:ARG:HH21	1.75	0.52
11:K:18:ARG:HA	11:K:81:ASP:H	1.75	0.52
12:L:53:ARG:HG2	12:L:53:ARG:NH1	2.21	0.52
15:O:62:GLN:HA	15:O:65:ARG:NH1	2.25	0.52
17:Q:92:ARG:HG2	17:Q:92:ARG:O	2.10	0.52
23:Y:39:A:H3'	23:Y:40:U:H6	1.74	0.52
1:A:474:G:C5'	1:A:474:G:C4	2.93	0.52
1:A:976:G:C8	1:A:1358:U:C2	2.98	0.52
1:A:1201:A:H4'	1:A:1202:G:H5"	1.91	0.52
2:B:80:ILE:HD11	2:B:208:ILE:CG2	2.26	0.52
3:C:60:ALA:O	3:C:61:ALA:HB2	2.10	0.52
9:I:84:ALA:C	9:I:86:VAL:H	2.13	0.52
10:J:24:VAL:HG12	10:J:24:VAL:O	2.10	0.52
17:Q:59:ILE:HG22	17:Q:71:PHE:CD1	2.45	0.52
1:A:523:A:C6	12:L:92:ASP:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:G:H4'	1:A:994:A:OP2	2.10	0.52
2:B:197:VAL:HG12	2:B:200:ILE:HG13	1.91	0.52
3:C:18:TRP:HB3	14:N:51:GLY:O	2.10	0.52
3:C:152:ILE:CG2	3:C:153:VAL:N	2.73	0.52
4:D:162:LEU:HD21	4:D:178:VAL:O	2.10	0.52
18:R:52:PRO:O	18:R:56:THR:HG23	2.10	0.52
1:A:54:C:H2'	1:A:352:C:H41	1.76	0.51
1:A:61:G:H2'	1:A:62:U:O4'	2.10	0.51
1:A:371:G:C2'	1:A:372:C:H5'	2.40	0.51
1:A:730:G:H2'	1:A:731:G:H5'	1.92	0.51
1:A:1030(D):A:H2'	1:A:1031:G:C4'	2.40	0.51
3:C:8:ILE:O	3:C:11:ARG:N	2.39	0.51
3:C:35:GLU:OE2	3:C:59:ARG:NH2	2.38	0.51
7:G:148:ASN:C	7:G:150:ALA:H	2.14	0.51
9:I:85:LEU:HB3	9:I:92:TYR:CD1	2.44	0.51
12:L:29:GLY:O	12:L:30:ALA:C	2.47	0.51
1:A:191:G:C8	1:A:191:G:C5'	2.93	0.51
1:A:673:G:H5"	6:F:87:ARG:CZ	2.41	0.51
1:A:912:C:H5"	12:L:46:LYS:NZ	2.25	0.51
2:B:58:ILE:HG23	2:B:68:ILE:HD12	1.92	0.51
2:B:165:VAL:O	2:B:187:LEU:O	2.29	0.51
7:G:74:GLU:O	7:G:88:PRO:HA	2.10	0.51
7:G:75:VAL:CG1	7:G:86:GLN:HB3	2.33	0.51
10:J:20:ALA:HA	10:J:23:ILE:HD12	1.91	0.51
11:K:32:ILE:O	11:K:40:ILE:HB	2.10	0.51
17:Q:65:ILE:HG21	17:Q:69:LYS:NZ	2.25	0.51
20:T:87:LYS:O	20:T:91:LEU:HB2	2.10	0.51
1:A:1158:C:H5"	2:B:133:LYS:NZ	2.26	0.51
1:A:1397:C:H42	22:X:4:G:H2'	1.74	0.51
1:A:1503:A:C5'	1:A:1531:A:H1'	2.41	0.51
3:C:112:SER:O	3:C:116:VAL:HG23	2.10	0.51
4:D:5:ILE:HG22	4:D:5:ILE:O	2.10	0.51
5:E:75:THR:HG23	5:E:76:ILE:O	2.09	0.51
8:H:45:ILE:HA	8:H:64:LYS:HG2	1.92	0.51
9:I:19:LEU:HB3	9:I:59:PHE:HD2	1.73	0.51
9:I:97:LYS:HA	9:I:102:LEU:HD21	1.91	0.51
1:A:397:A:H3'	1:A:397:A:N3	2.24	0.51
1:A:707:C:H4'	11:K:20:TYR:HD1	1.70	0.51
1:A:1067:A:N3	1:A:1068:G:H1'	2.24	0.51
1:A:1343:G:H2'	1:A:1344:C:H6	1.74	0.51
1:A:1347:G:H2'	1:A:1373:G:O6	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1399:C:C2	1:A:1502:A:N6	2.78	0.51
6:F:67:MET:HB2	6:F:68:PRO:CD	2.41	0.51
16:P:33:ILE:O	16:P:34:GLU:HB2	2.09	0.51
18:R:55:ARG:CA	18:R:55:ARG:HH11	2.23	0.51
19:S:55:LYS:O	19:S:55:LYS:HG2	2.09	0.51
20:T:48:LYS:O	20:T:50:GLU:N	2.44	0.51
1:A:173:U:H5	1:A:198:G:HO2'	1.51	0.51
1:A:458:C:O2	1:A:458:C:C2'	2.59	0.51
1:A:994:A:N1	1:A:1047:G:H4'	2.26	0.51
1:A:1055:A:N3	3:C:156:ARG:HD2	2.25	0.51
2:B:82:ARG:CA	2:B:92:TYR:HE1	2.14	0.51
2:B:91:PRO:HG3	2:B:154:LEU:CD1	2.40	0.51
2:B:237:ALA:C	2:B:239:VAL:H	2.13	0.51
3:C:130:VAL:O	3:C:134:ILE:HG13	2.10	0.51
7:G:138:LYS:C	7:G:140:ASP:N	2.64	0.51
9:I:125:TYR:CD2	9:I:125:TYR:N	2.77	0.51
12:L:11:VAL:CG1	12:L:11:VAL:O	2.59	0.51
19:S:67:VAL:O	19:S:67:VAL:HG12	2.11	0.51
1:A:151:A:H2'	1:A:152:A:O4'	2.10	0.51
1:A:376:G:C2	1:A:389:A:C2	2.98	0.51
1:A:1436:U:H2'	1:A:1437:C:C6	2.44	0.51
2:B:213:LEU:O	2:B:216:SER:HB3	2.10	0.51
4:D:183:GLY:O	4:D:184:LYS:HB2	2.10	0.51
7:G:6:ARG:O	7:G:7:ALA:O	2.28	0.51
8:H:69:ARG:HG2	8:H:70:GLN:N	2.25	0.51
9:I:111:ARG:HD2	14:N:61:TRP:OXT	2.11	0.51
13:M:66:LEU:HA	13:M:70:LEU:HD12	1.93	0.51
1:A:386:C:C2'	1:A:387:U:H5'	2.41	0.51
1:A:445:G:H2'	1:A:446:G:C8	2.46	0.51
1:A:518:C:H5'	1:A:530:G:O4'	2.10	0.51
1:A:532:A:H62	3:C:161:GLU:HB3	1.73	0.51
1:A:1352:C:H2'	1:A:1353:G:C8	2.46	0.51
6:F:69:GLU:C	6:F:71:ARG:H	2.14	0.51
15:O:17:ARG:CZ	15:O:77:ARG:HD3	2.40	0.51
1:A:6:G:H4'	1:A:298:A:H4'	1.92	0.51
1:A:154:C:H2'	1:A:155:C:C6	2.46	0.51
1:A:189:G:O2'	1:A:190:C:O5'	2.28	0.51
1:A:513:C:H2'	1:A:514:C:H6	1.76	0.51
1:A:1004:A:H1'	1:A:1036:G:N1	2.21	0.51
1:A:1118:C:H1'	1:A:1179:A:C4	2.45	0.51
1:A:1164:G:H2'	1:A:1165:C:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:G:O2'	1:A:1273:G:H5'	2.11	0.51
4:D:149:ALA:O	4:D:152:SER:HB2	2.11	0.51
15:O:10:LYS:HD2	15:O:10:LYS:O	2.10	0.51
20:T:11:SER:N	20:T:13:LEU:CD1	2.74	0.51
1:A:76:C:H42	1:A:93:G:N2	2.08	0.51
1:A:175:C:O2'	1:A:176:C:H5'	2.11	0.51
1:A:403:C:O3'	4:D:122:ARG:HD3	2.11	0.51
1:A:523:A:H61	12:L:53:ARG:HH12	1.57	0.51
1:A:603:U:H2'	1:A:604:G:H8	1.75	0.51
1:A:674:G:H2'	1:A:675:A:H8	1.75	0.51
1:A:1004:A:H3'	1:A:1004:A:N3	2.25	0.51
1:A:1346:A:O4'	1:A:1348:U:C6	2.64	0.51
2:B:25:ASN:C	2:B:25:ASN:ND2	2.64	0.51
2:B:105:PHE:CE1	2:B:155:LEU:HD22	2.46	0.51
2:B:209:ARG:HH21	2:B:239:VAL:HG11	1.76	0.51
3:C:88:ARG:HG3	3:C:101:LEU:HB3	1.93	0.51
4:D:131:ARG:HD2	4:D:131:ARG:H	1.74	0.51
13:M:14:ARG:H	13:M:44:ARG:NH2	2.04	0.51
15:O:87:ILE:HG22	15:O:88:ARG:N	2.26	0.51
4:D:165:MET:SD	4:D:168:ARG:HD3	2.51	0.51
6:F:11:ASN:ND2	6:F:86:ARG:NH2	2.59	0.51
13:M:73:GLU:O	13:M:77:ASN:HB2	2.11	0.51
19:S:11:VAL:HG13	19:S:38:SER:HB2	1.92	0.51
1:A:28:G:O2'	1:A:296:U:OP1	2.29	0.50
1:A:359:U:H2'	1:A:360:A:C8	2.42	0.50
1:A:477:G:H2'	1:A:477:G:N3	2.26	0.50
1:A:841:U:H3	2:B:37:ASN:HA	1.75	0.50
6:F:5:GLU:O	6:F:90:VAL:HA	2.11	0.50
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.93	0.50
9:I:69:GLY:O	9:I:73:GLN:HG3	2.10	0.50
9:I:118:LYS:HB2	9:I:118:LYS:HZ2	1.76	0.50
10:J:45:ARG:NH2	14:N:36:PHE:HB2	2.26	0.50
19:S:33:THR:HG22	19:S:34:TRP:N	2.27	0.50
19:S:58:VAL:O	19:S:60:VAL:HG23	2.11	0.50
1:A:263:A:H2'	1:A:264:U:C5	2.46	0.50
1:A:562:C:H1'	12:L:15:ARG:HB3	1.91	0.50
1:A:649:G:O2'	1:A:650:G:H5'	2.11	0.50
1:A:895:G:H2'	1:A:896:C:C6	2.46	0.50
1:A:1221:G:O3'	19:S:77:THR:OG1	2.28	0.50
1:A:1325:C:O3'	21:V:17:THR:HG21	2.10	0.50
1:A:1374:A:C4	1:A:1375:A:C8	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:G:OP2	1:A:1447:G:OP2	2.28	0.50
5:E:37:ARG:HG2	5:E:37:ARG:HH11	1.76	0.50
20:T:10:LEU:O	20:T:12:ALA:N	2.44	0.50
1:A:949:A:C2	1:A:1233:G:N3	2.79	0.50
1:A:1068:G:OP2	1:A:1068:G:H8	1.94	0.50
1:A:1447:G:N1	1:A:1460:A:C2	2.73	0.50
7:G:25:ALA:HA	7:G:28:ASN:HD22	1.76	0.50
8:H:45:ILE:O	8:H:46:LYS:C	2.50	0.50
10:J:82:ILE:HG22	10:J:86:MET:SD	2.52	0.50
12:L:33:ARG:CG	12:L:60:LEU:HD12	2.41	0.50
18:R:39:VAL:CG1	18:R:40:LEU:N	2.73	0.50
19:S:29:ARG:O	19:S:30:LEU:HB3	2.11	0.50
1:A:84:U:H2'	1:A:88:A:C8	2.46	0.50
1:A:1044:A:H2'	1:A:1045:C:O4'	2.11	0.50
1:A:1226:C:O3'	13:M:111:LYS:HE2	2.11	0.50
2:B:12:GLU:C	2:B:14:GLY:N	2.65	0.50
2:B:137:ARG:HD3	2:B:138:LEU:HG	1.93	0.50
5:E:21:ALA:O	5:E:23:GLY:N	2.39	0.50
12:L:85:ILE:CG2	12:L:98:TYR:HB3	2.41	0.50
12:L:90:VAL:CG1	12:L:93:LEU:HD21	2.42	0.50
15:O:39:LEU:HD13	15:O:43:LEU:HG	1.93	0.50
17:Q:24:GLU:HA	17:Q:39:SER:CB	2.39	0.50
1:A:939:G:H2'	1:A:940:C:C6	2.46	0.50
1:A:962:C:H42	1:A:973:G:H1	1.59	0.50
1:A:1459:C:C2	1:A:1460:A:C8	2.99	0.50
4:D:8:VAL:O	4:D:10:ARG:N	2.44	0.50
5:E:96:PRO:HA	5:E:117:ASP:OD2	2.11	0.50
6:F:38:GLU:O	6:F:39:LYS:C	2.50	0.50
10:J:4:ILE:CD1	10:J:74:ILE:HB	2.31	0.50
13:M:14:ARG:NH1	13:M:16:ASP:OD2	2.45	0.50
13:M:40:ASN:HD22	13:M:41:PRO:CD	2.24	0.50
16:P:26:ARG:HD3	16:P:31:LYS:O	2.12	0.50
18:R:40:LEU:O	18:R:41:LYS:C	2.50	0.50
1:A:67:C:O2'	1:A:171:A:H1'	2.11	0.50
1:A:377:G:O2'	1:A:378:G:H5'	2.10	0.50
1:A:581:G:O3'	15:O:64:ARG:NH2	2.44	0.50
1:A:591:U:H2'	1:A:592:G:H8	1.77	0.50
1:A:666:G:H5'	1:A:726:C:H1'	1.93	0.50
1:A:712:A:H2'	1:A:713:G:O4'	2.12	0.50
1:A:841:U:N3	2:B:37:ASN:HA	2.26	0.50
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:G:H5"	10:J:35:SER:HA	1.93	0.50
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.45	0.50
2:B:118:LEU:HB2	2:B:142:LEU:HD21	1.93	0.50
5:E:107:ARG:O	5:E:110:LEU:N	2.42	0.50
9:I:127:LYS:H	9:I:127:LYS:CD	2.22	0.50
1:A:113:G:O2'	1:A:114:U:H5'	2.12	0.50
1:A:304:U:H2'	1:A:305:G:C8	2.46	0.50
1:A:376:G:P	16:P:67:THR:HG21	2.52	0.50
1:A:1004:A:N7	1:A:1005:A:N3	2.60	0.50
1:A:1138:G:H3'	1:A:1138:G:N3	2.27	0.50
1:A:1288:A:H1'	1:A:1352:C:O2'	2.11	0.50
1:A:1474:G:H2'	1:A:1475:G:H8	1.77	0.50
2:B:17:PHE:CD1	2:B:17:PHE:C	2.85	0.50
3:C:43:LEU:HD23	3:C:43:LEU:C	2.32	0.50
3:C:54:ARG:HG2	3:C:56:ASP:OD1	2.12	0.50
5:E:11:ILE:HD11	5:E:33:VAL:CG2	2.42	0.50
8:H:4:ASP:OD2	8:H:7:ALA:HB2	2.11	0.50
12:L:41:ARG:CG	12:L:42:THR:H	2.05	0.50
12:L:62:SER:O	12:L:64:TYR:HD1	1.95	0.50
14:N:7:ILE:O	14:N:7:ILE:HG22	2.11	0.50
19:S:64:GLU:O	19:S:66:MET:N	2.45	0.50
1:A:353:A:H5'	1:A:353:A:C8	2.47	0.50
1:A:1005:A:H1'	1:A:1036:G:N2	2.27	0.50
2:B:230:VAL:HG13	2:B:231:GLU:OE2	2.12	0.50
9:I:113:LYS:H	9:I:113:LYS:HD2	1.76	0.50
10:J:4:ILE:HD12	10:J:74:ILE:CB	2.32	0.50
10:J:9:ARG:O	10:J:16:LEU:HD11	2.12	0.50
12:L:46:LYS:HE2	12:L:47:LYS:HE3	1.94	0.50
13:M:2:ALA:C	13:M:9:ILE:HG23	2.32	0.50
14:N:42:ILE:O	14:N:46:GLU:HG3	2.11	0.50
15:O:53:HIS:CE1	15:O:57:LEU:HD11	2.46	0.50
19:S:18:LYS:O	19:S:22:LEU:HG	2.12	0.50
19:S:52:TYR:HB2	19:S:57:HIS:CE1	2.47	0.50
1:A:184:G:H2'	1:A:185:A:H8	1.77	0.50
1:A:437:U:H3	1:A:496:A:H62	1.57	0.50
1:A:545:C:O2'	1:A:546:G:H5'	2.11	0.50
1:A:1375:A:H2'	1:A:1376:U:C6	2.47	0.50
2:B:12:GLU:O	2:B:14:GLY:N	2.44	0.50
2:B:116:GLU:HG2	2:B:153:ARG:NH2	2.26	0.50
2:B:230:VAL:HG12	2:B:231:GLU:N	2.27	0.50
5:E:101:ILE:HG22	5:E:101:ILE:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:102:ALA:HB1	5:E:106:PRO:HB2	1.94	0.50
7:G:47:CYS:HA	7:G:50:ILE:CD1	2.41	0.50
15:O:77:ARG:O	15:O:80:ALA:HB3	2.12	0.50
15:O:84:LYS:O	15:O:84:LYS:HG2	2.12	0.50
1:A:530:G:C6	22:X:3:G:H8	2.30	0.49
1:A:605:U:H2'	1:A:606:G:O4'	2.12	0.49
1:A:1054:C:C4	23:Y:35:C:O4'	2.65	0.49
1:A:1268:A:H1'	1:A:1326:C:O2'	2.12	0.49
1:A:1301:U:O2'	1:A:1302:U:OP1	2.29	0.49
1:A:1508:G:H2'	1:A:1509:C:H6	1.76	0.49
4:D:83:SER:HA	4:D:89:THR:OG1	2.12	0.49
4:D:127:THR:HG22	4:D:130:GLY:H	1.77	0.49
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.27	0.49
9:I:10:ARG:HD2	9:I:11:LYS:H	1.76	0.49
11:K:54:ARG:HH11	11:K:54:ARG:CB	2.24	0.49
13:M:8:GLU:C	13:M:9:ILE:HD12	2.32	0.49
13:M:23:TYR:HE2	13:M:70:LEU:HD22	1.76	0.49
18:R:58:LEU:HD22	18:R:62:GLU:HB3	1.93	0.49
19:S:81:ARG:O	19:S:81:ARG:HG2	2.12	0.49
1:A:358:U:O2'	1:A:359:U:H5'	2.12	0.49
1:A:418:C:O2'	1:A:419:C:H5'	2.12	0.49
1:A:529:G:C4'	1:A:533:A:C2	2.95	0.49
1:A:640:A:C2'	1:A:641:U:H5'	2.42	0.49
1:A:1260:C:H4'	1:A:1284:C:H5'	1.93	0.49
1:A:1329:A:O2'	1:A:1330:U:H5'	2.12	0.49
2:B:184:VAL:N	2:B:198:ASP:OD2	2.45	0.49
4:D:62:GLN:HE21	4:D:62:GLN:CA	2.13	0.49
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.94	0.49
5:E:129:ILE:HD12	5:E:129:ILE:N	2.16	0.49
8:H:38:ILE:N	8:H:38:ILE:HD12	2.26	0.49
8:H:112:LEU:HD23	8:H:119:LEU:O	2.13	0.49
9:I:25:LYS:HG2	9:I:60:ASP:OD1	2.12	0.49
9:I:40:LEU:C	9:I:42:ARG:H	2.14	0.49
12:L:117:ARG:HH21	12:L:124:LYS:HA	1.76	0.49
20:T:12:ALA:O	20:T:15:ARG:HB2	2.12	0.49
20:T:72:LEU:O	20:T:73:HIS:O	2.30	0.49
1:A:317:G:C6	1:A:318:G:N7	2.80	0.49
1:A:504:C:H2'	1:A:511:C:H5	1.77	0.49
1:A:1333:A:H2'	1:A:1334:G:O4'	2.13	0.49
1:A:1413:A:H2	1:A:1487:G:H22	1.56	0.49
1:A:1424:C:H2'	1:A:1425:U:H6	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:GLU:HA	2:B:39:ILE:O	2.11	0.49
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.94	0.49
2:B:194:PRO:O	2:B:196:LEU:N	2.46	0.49
3:C:2:GLY:O	3:C:4:LYS:N	2.45	0.49
3:C:67:THR:O	3:C:67:THR:HG22	2.12	0.49
3:C:112:SER:HB2	3:C:115:LEU:HD12	1.95	0.49
6:F:75:LEU:O	6:F:75:LEU:HD13	2.11	0.49
7:G:38:LEU:C	7:G:38:LEU:HD12	2.33	0.49
9:I:10:ARG:HD2	9:I:11:LYS:N	2.28	0.49
9:I:97:LYS:O	9:I:100:GLY:N	2.45	0.49
18:R:39:VAL:HG13	18:R:40:LEU:H	1.77	0.49
20:T:16:HIS:HE1	20:T:20:LEU:HD21	1.77	0.49
20:T:36:LEU:HD21	20:T:58:LYS:HD3	1.94	0.49
20:T:75:ASN:N	20:T:75:ASN:OD1	2.44	0.49
1:A:56:U:H2'	1:A:57:G:C8	2.47	0.49
1:A:376:G:N3	1:A:389:A:C2	2.80	0.49
1:A:687:A:H2'	1:A:701:C:H41	1.77	0.49
1:A:1130:A:H62	1:A:1144:G:H21	1.58	0.49
1:A:1214:C:H5"	1:A:1215:G:OP2	2.12	0.49
3:C:180:ALA:C	3:C:182:ILE:H	2.15	0.49
4:D:104:VAL:CG1	4:D:146:ILE:HD12	2.41	0.49
5:E:105:VAL:O	5:E:106:PRO:C	2.50	0.49
8:H:104:ARG:O	8:H:105:ARG:C	2.50	0.49
14:N:18:VAL:O	14:N:18:VAL:HG23	2.11	0.49
17:Q:101:ARG:HA	17:Q:101:ARG:HE	1.78	0.49
1:A:757:U:H2'	1:A:758:G:O4'	2.11	0.49
1:A:829:G:O2'	1:A:830:G:H5'	2.13	0.49
1:A:1219:U:O2'	19:S:34:TRP:HB3	2.12	0.49
1:A:1367:C:C2	1:A:1368:G:C8	3.01	0.49
2:B:93:VAL:HG11	2:B:97:TRP:HA	1.93	0.49
3:C:75:VAL:HG12	3:C:83:ARG:CZ	2.41	0.49
6:F:19:LEU:C	6:F:19:LEU:HD23	2.32	0.49
7:G:18:TYR:HD2	7:G:59:LEU:HD13	1.77	0.49
12:L:34:ARG:HB3	12:L:61:THR:HG21	1.93	0.49
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.12	0.49
1:A:1003:G:N2	1:A:1004:A:O2'	2.45	0.49
1:A:1505:G:C8	1:A:1505:G:H3'	2.47	0.49
2:B:15:VAL:HG11	2:B:209:ARG:HG3	1.94	0.49
2:B:19:HIS:CD2	2:B:189:ASP:HB2	2.41	0.49
2:B:240:GLN:CD	2:B:240:GLN:N	2.66	0.49
3:C:180:ALA:C	3:C:182:ILE:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:15:ASP:OD1	6:F:17:SER:HB2	2.13	0.49
6:F:18:GLN:HA	6:F:21:LEU:CB	2.35	0.49
6:F:101:ALA:HA	18:R:28:GLU:HG3	1.95	0.49
8:H:96:GLY:H	8:H:99:GLU:HB2	1.76	0.49
13:M:87:TYR:C	13:M:89:GLY:N	2.65	0.49
1:A:296:U:H2'	1:A:297:G:H8	1.77	0.49
1:A:357:G:OP1	1:A:367:U:H5"	2.13	0.49
1:A:524:G:H2'	1:A:525:C:C5	2.46	0.49
1:A:989:C:H42	1:A:1216:G:H1	1.61	0.49
1:A:1273:G:H2'	1:A:1274:G:O4'	2.12	0.49
4:D:3:ARG:CZ	4:D:118:ARG:NH1	2.76	0.49
4:D:13:ARG:HG3	4:D:32:ALA:HB1	1.94	0.49
4:D:64:LEU:HD11	4:D:97:LEU:HD11	1.95	0.49
9:I:24:GLY:O	9:I:26:VAL:N	2.45	0.49
9:I:40:LEU:O	9:I:42:ARG:N	2.45	0.49
9:I:53:VAL:HG11	9:I:92:TYR:CE2	2.48	0.49
12:L:28:LYS:O	12:L:28:LYS:HG2	2.13	0.49
12:L:69:TYR:HB2	12:L:90:VAL:HG21	1.95	0.49
17:Q:101:ARG:HD3	17:Q:102:GLY:N	2.28	0.49
1:A:279:A:H5"	1:A:280:C:H3'	1.93	0.49
1:A:389:A:H2'	1:A:390:C:C5'	2.43	0.49
1:A:974:A:H8	1:A:974:A:OP1	1.95	0.49
1:A:1427:U:H2'	1:A:1428:A:H8	1.78	0.49
3:C:44:GLU:C	3:C:46:GLU:H	2.15	0.49
6:F:35:ALA:HB1	6:F:65:VAL:CG1	2.40	0.49
10:J:22:LYS:C	10:J:24:VAL:N	2.65	0.49
12:L:68:ALA:HB1	12:L:100:ILE:HG13	1.94	0.49
17:Q:67:LYS:CA	17:Q:70:ARG:HH12	2.24	0.49
1:A:138:G:O2'	1:A:139:G:H5'	2.13	0.49
1:A:952:U:O4	13:M:104:ARG:HD3	2.13	0.49
1:A:1004:A:OP1	1:A:1025:U:O2	2.31	0.49
1:A:1200:C:H1'	1:A:1204:A:N6	2.27	0.49
1:A:1327:C:H2'	1:A:1328:C:C6	2.47	0.49
1:A:1429:C:H2'	1:A:1430:C:C6	2.48	0.49
2:B:19:HIS:NE2	2:B:20:GLU:OE2	2.46	0.49
2:B:141:GLU:O	2:B:143:GLU:N	2.46	0.49
3:C:36:ASP:HA	3:C:39:ILE:HB	1.95	0.49
3:C:110:ASN:C	3:C:112:SER:H	2.16	0.49
5:E:75:THR:HG23	5:E:76:ILE:N	2.28	0.49
7:G:16:LEU:H	7:G:16:LEU:CD2	2.20	0.49
8:H:21:LYS:O	8:H:65:TYR:OH	2.17	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:65:TYR:N	8:H:65:TYR:CD1	2.81	0.49
9:I:118:LYS:O	9:I:119:ALA:HB3	2.13	0.49
16:P:55:ARG:O	16:P:56:ALA:C	2.51	0.49
1:A:428:G:H5'	1:A:430:A:O4'	2.13	0.49
1:A:710:G:H5"	6:F:54:LYS:NZ	2.28	0.49
1:A:818:G:O2'	1:A:819:A:H5'	2.12	0.49
1:A:1205:U:H4'	3:C:195:VAL:HG21	1.95	0.49
1:A:1316:G:H22	1:A:1319:A:P	2.36	0.49
1:A:1425:U:H2'	1:A:1426:C:C6	2.48	0.49
2:B:137:ARG:NH1	2:B:138:LEU:HD21	2.28	0.49
3:C:180:ALA:HB1	3:C:182:ILE:HG13	1.95	0.49
5:E:37:ARG:HG2	5:E:37:ARG:NH1	2.28	0.49
7:G:140:ASP:O	7:G:143:ARG:HB3	2.13	0.49
8:H:78:GLN:O	8:H:81:HIS:CE1	2.66	0.49
13:M:40:ASN:HD22	13:M:40:ASN:C	2.15	0.49
14:N:35:ARG:C	14:N:37:PHE:H	2.16	0.49
16:P:42:ARG:O	16:P:43:LYS:C	2.51	0.49
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.94	0.49
1:A:62:U:H2'	1:A:63:C:C5'	2.42	0.48
1:A:175:C:H2'	1:A:176:C:C6	2.40	0.48
1:A:386:C:O2'	1:A:387:U:H5'	2.12	0.48
1:A:514:C:H2'	1:A:515:G:C8	2.47	0.48
1:A:951:G:O2'	1:A:952:U:H5'	2.13	0.48
1:A:967:C:O2'	9:I:128:ARG:NH1	2.46	0.48
5:E:70:PRO:O	5:E:77:PRO:HD3	2.12	0.48
5:E:77:PRO:O	5:E:78:HIS:HB3	2.13	0.48
5:E:127:ASN:OD1	5:E:130:ASN:HB2	2.13	0.48
7:G:15:ASP:HB2	7:G:20:ASP:O	2.13	0.48
7:G:38:LEU:O	7:G:38:LEU:HD12	2.12	0.48
10:J:13:HIS:HB3	10:J:68:HIS:NE2	2.27	0.48
10:J:69:ASN:O	10:J:70:ARG:HD3	2.13	0.48
10:J:90:LEU:N	10:J:91:PRO:CD	2.62	0.48
15:O:54:ARG:O	15:O:58:MET:HG2	2.13	0.48
1:A:625:G:H2'	1:A:626:U:H6	1.76	0.48
1:A:891:U:O2'	1:A:892:A:H5'	2.12	0.48
1:A:1052:U:OP1	23:Y:34:C:C4	2.66	0.48
1:A:1152:A:H4'	10:J:17:ASP:OD2	2.14	0.48
1:A:1207:G:H2'	1:A:1208:C:H6	1.77	0.48
1:A:1374:A:O2'	1:A:1375:A:H5'	2.14	0.48
2:B:114:ARG:C	2:B:116:GLU:N	2.66	0.48
2:B:167:PRO:HG2	2:B:192:SER:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:ARG:O	2:B:220:ASP:N	2.46	0.48
3:C:147:LYS:HE2	3:C:205:GLY:HA2	1.95	0.48
3:C:169:ALA:O	3:C:170:GLN:HB2	2.12	0.48
3:C:179:ARG:HD2	3:C:206:GLU:HG3	1.95	0.48
9:I:113:LYS:HD2	9:I:113:LYS:N	2.27	0.48
13:M:4:ILE:HG22	13:M:5:ALA:N	2.27	0.48
13:M:14:ARG:HB3	13:M:16:ASP:OD1	2.13	0.48
16:P:8:ARG:CZ	16:P:15:PRO:HB3	2.43	0.48
18:R:62:GLU:O	18:R:64:ARG:N	2.47	0.48
1:A:521:G:OP1	12:L:73:GLU:O	2.32	0.48
1:A:707:C:H4'	11:K:20:TYR:CE1	2.47	0.48
3:C:84:ILE:HG12	3:C:88:ARG:CD	2.33	0.48
7:G:21:VAL:C	7:G:23:VAL:N	2.65	0.48
8:H:45:ILE:O	8:H:45:ILE:CG1	2.61	0.48
12:L:50:SER:O	12:L:51:ALA:HB2	2.12	0.48
17:Q:9:VAL:HG21	17:Q:84:LEU:HD13	1.96	0.48
1:A:376:G:C4	1:A:389:A:C2	3.01	0.48
1:A:513:C:H2'	1:A:514:C:C6	2.48	0.48
1:A:877:C:H1'	8:H:3:THR:CG2	2.43	0.48
1:A:1117:G:N2	1:A:1180:A:H1'	2.28	0.48
1:A:1357:A:H2'	1:A:1358:U:C6	2.49	0.48
1:A:1365:G:C6	1:A:1366:C:C4	3.01	0.48
2:B:36:ARG:HB2	2:B:41:ILE:HD12	1.94	0.48
2:B:103:THR:HA	2:B:180:LEU:HD11	1.95	0.48
4:D:4:TYR:O	4:D:5:ILE:HB	2.12	0.48
20:T:71:THR:O	20:T:72:LEU:HD23	2.14	0.48
1:A:242:C:H2'	1:A:243:A:H5'	1.94	0.48
1:A:489:C:H2'	1:A:490:G:C8	2.39	0.48
1:A:519:C:H2'	1:A:520:A:C8	2.49	0.48
1:A:522:C:N4	12:L:53:ARG:HH22	1.92	0.48
1:A:934:C:H5	1:A:1344:C:H2'	1.78	0.48
1:A:1237:C:C4'	1:A:1334:G:N2	2.77	0.48
1:A:1298:C:H2'	7:G:114:ARG:NH2	2.28	0.48
1:A:1392:G:H2'	1:A:1393:U:H6	1.79	0.48
3:C:140:ARG:HG3	3:C:141:VAL:H	1.79	0.48
9:I:64:THR:CG2	9:I:66:ARG:HH12	2.26	0.48
10:J:30:SER:HB2	10:J:80:LYS:O	2.14	0.48
12:L:27:LEU:C	12:L:29:GLY:N	2.67	0.48
12:L:111:LYS:O	12:L:112:ASP:CB	2.61	0.48
13:M:22:ILE:O	13:M:23:TYR:O	2.31	0.48
15:O:4:THR:HB	15:O:6:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:C:H2'	1:A:132:C:C6	2.48	0.48
1:A:381:C:H2'	1:A:382:A:H5'	1.95	0.48
1:A:624:C:O2'	1:A:625:G:H5'	2.14	0.48
1:A:674:G:H4'	18:R:81:PHE:CD1	2.48	0.48
1:A:724:G:O2'	1:A:725:G:H5'	2.13	0.48
1:A:991:U:HO2'	1:A:993:G:H8	1.56	0.48
1:A:1074:G:O2'	2:B:103:THR:HG22	2.13	0.48
1:A:1347:G:H1'	1:A:1348:U:H5	1.78	0.48
1:A:1419:G:H2'	1:A:1420:C:C6	2.48	0.48
1:A:1447:G:O6	1:A:1460:A:C6	2.66	0.48
3:C:117:ALA:CB	3:C:187:ALA:HB2	2.40	0.48
4:D:91:SER:OG	4:D:92:VAL:N	2.47	0.48
6:F:75:LEU:O	6:F:79:LEU:HD12	2.13	0.48
8:H:91:ARG:HG3	12:L:7:ILE:HG13	1.96	0.48
15:O:82:ILE:C	15:O:84:LYS:H	2.15	0.48
19:S:30:LEU:HD22	19:S:31:ILE:N	2.28	0.48
1:A:46:G:O2'	1:A:365:U:H1'	2.13	0.48
1:A:392:G:H2'	1:A:393:A:C8	2.49	0.48
1:A:537:G:OP1	12:L:113:ARG:NH2	2.44	0.48
1:A:539:A:H2'	1:A:540:G:C8	2.49	0.48
1:A:574:A:N3	1:A:883:C:H1'	2.28	0.48
1:A:848:C:H5"	2:B:22:LYS:NZ	2.29	0.48
1:A:1504:G:H4'	1:A:1505:G:H5'	1.95	0.48
4:D:10:ARG:HG2	4:D:10:ARG:HH11	1.78	0.48
4:D:77:ASN:O	4:D:81:GLU:HB2	2.14	0.48
4:D:135:LEU:HB2	4:D:138:TYR:HB2	1.96	0.48
6:F:6:VAL:O	6:F:8:ILE:HG13	2.13	0.48
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.49	0.48
8:H:133:LEU:C	8:H:133:LEU:HD23	2.34	0.48
13:M:121:LYS:N	13:M:121:LYS:HD2	2.29	0.48
19:S:39:THR:HG22	19:S:40:ILE:N	2.28	0.48
19:S:44:MET:O	19:S:62:ILE:HG21	2.14	0.48
20:T:76:ALA:O	20:T:80:ARG:HG3	2.13	0.48
1:A:9:G:C2	1:A:26:A:C2	3.02	0.48
1:A:335:C:H2'	1:A:336:C:H6	1.79	0.48
1:A:953:G:H1'	13:M:125:ARG:HA	1.96	0.48
1:A:959:A:C3'	1:A:960:U:H4'	2.43	0.48
1:A:1131:G:H1	1:A:1143:G:H21	1.61	0.48
1:A:1375:A:H2'	1:A:1376:U:H6	1.77	0.48
2:B:189:ASP:N	2:B:189:ASP:OD1	2.46	0.48
2:B:233:SER:OG	2:B:234:PRO:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:138:VAL:CG2	3:C:168:ALA:HB1	2.43	0.48
5:E:116:THR:HG23	5:E:117:ASP:H	1.79	0.48
10:J:7:LYS:HZ3	10:J:99:LYS:HD2	1.79	0.48
10:J:12:ASP:HB3	10:J:15:THR:HG22	1.94	0.48
10:J:20:ALA:HA	10:J:23:ILE:HB	1.95	0.48
12:L:29:GLY:O	12:L:30:ALA:O	2.31	0.48
13:M:4:ILE:CD1	13:M:19:LEU:HD21	2.44	0.48
18:R:22:VAL:O	18:R:22:VAL:HG12	2.13	0.48
19:S:11:VAL:HG22	19:S:39:THR:H	1.79	0.48
1:A:167:G:H2'	1:A:168:G:H8	1.78	0.48
1:A:708:C:H2'	1:A:709:G:C8	2.49	0.48
1:A:1178:G:N2	1:A:1180:A:H3'	2.28	0.48
1:A:1346:A:C4	7:G:10:ARG:NH2	2.82	0.48
2:B:18:GLY:O	2:B:204:ASN:ND2	2.46	0.48
2:B:102:LEU:N	2:B:102:LEU:HD12	2.29	0.48
3:C:27:LYS:CB	3:C:30:ARG:HH22	2.26	0.48
3:C:47:LEU:CD2	3:C:68:VAL:HG11	2.44	0.48
6:F:91:VAL:O	6:F:91:VAL:HG13	2.12	0.48
10:J:40:LEU:HD23	10:J:69:ASN:CB	2.43	0.48
12:L:83:VAL:HG21	12:L:100:ILE:CG2	2.43	0.48
18:R:45:SER:C	18:R:47:THR:N	2.65	0.48
20:T:16:HIS:O	20:T:19:SER:HB3	2.14	0.48
20:T:83:ARG:HB2	20:T:87:LYS:NZ	2.29	0.48
1:A:243:A:C2	1:A:246:A:C8	3.01	0.48
1:A:442:C:H5	1:A:443:C:H41	1.61	0.48
2:B:7:VAL:HG23	2:B:7:VAL:O	2.13	0.48
3:C:95:THR:O	3:C:97:LYS:HG2	2.14	0.48
4:D:38:TYR:HB2	4:D:39:PRO:HD2	1.96	0.48
4:D:87:GLY:O	4:D:89:THR:N	2.47	0.48
8:H:25:ASP:OD1	8:H:25:ASP:N	2.46	0.48
9:I:58:ARG:HH11	9:I:58:ARG:HG3	1.78	0.48
10:J:5:ARG:CD	10:J:99:LYS:HB2	2.44	0.48
20:T:39:LYS:HE2	20:T:55:ILE:CD1	2.41	0.48
20:T:79:ARG:HH11	20:T:79:ARG:HG3	1.78	0.48
21:V:2:GLY:C	21:V:4:GLY:H	2.17	0.48
1:A:12:U:H4'	1:A:526:C:O2'	2.14	0.47
1:A:376:G:O2'	1:A:377:G:H5'	2.14	0.47
1:A:708:C:H2'	1:A:709:G:H8	1.78	0.47
1:A:942:G:H2'	1:A:943:U:H6	1.79	0.47
1:A:1288:A:N1	1:A:1371:G:H1'	2.29	0.47
1:A:1347:G:C2'	1:A:1348:U:OP2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ARG:C	2:B:84:GLU:H	2.17	0.47
3:C:95:THR:O	3:C:97:LYS:N	2.47	0.47
4:D:56:VAL:O	4:D:57:ARG:C	2.52	0.47
4:D:157:LEU:HD23	4:D:157:LEU:C	2.34	0.47
5:E:60:TYR:O	5:E:64:ARG:HG2	2.14	0.47
8:H:14:ARG:NH1	8:H:14:ARG:HB2	2.29	0.47
9:I:42:ARG:HB2	9:I:74:ILE:HD13	1.94	0.47
12:L:38:THR:HG22	12:L:39:VAL:CG1	2.44	0.47
15:O:62:GLN:HA	15:O:65:ARG:HH12	1.79	0.47
16:P:45:THR:O	16:P:48:TRP:HD1	1.97	0.47
20:T:24:LEU:HD12	20:T:24:LEU:O	2.13	0.47
1:A:35:G:H21	12:L:118:SER:HB2	1.77	0.47
1:A:523:A:N6	12:L:53:ARG:HH12	2.12	0.47
1:A:794:A:H2'	1:A:795:C:H6	1.74	0.47
1:A:861:G:H2'	1:A:862:C:H6	1.79	0.47
1:A:925:G:C6	1:A:927:G:N7	2.82	0.47
1:A:996:A:O2'	1:A:997:U:H5'	2.15	0.47
1:A:1023:G:H2'	1:A:1023:G:N3	2.29	0.47
1:A:1057:G:H5"	3:C:154:SER:CB	2.44	0.47
1:A:1289:A:H2'	1:A:1290:G:H5'	1.96	0.47
2:B:100:GLY:O	2:B:104:ASN:N	2.45	0.47
3:C:201:TYR:N	3:C:201:TYR:CD1	2.82	0.47
4:D:177:ASP:OD1	4:D:177:ASP:O	2.32	0.47
5:E:41:VAL:HG13	5:E:113:ALA:CA	2.41	0.47
5:E:121:LYS:HE3	5:E:122:GLU:H	1.79	0.47
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.38	0.47
9:I:64:THR:O	9:I:65:VAL:C	2.52	0.47
10:J:71:LEU:O	10:J:72:VAL:HB	2.14	0.47
13:M:65:LYS:HG3	13:M:69:GLU:OE2	2.14	0.47
13:M:78:ILE:C	13:M:80:ARG:H	2.17	0.47
13:M:81:LEU:H	13:M:81:LEU:CD2	2.18	0.47
18:R:43:PHE:C	18:R:51:LEU:HD12	2.34	0.47
19:S:15:LEU:C	19:S:15:LEU:HD12	2.35	0.47
1:A:154:C:H2'	1:A:155:C:H6	1.78	0.47
1:A:197:A:H1'	1:A:198:G:O4'	2.14	0.47
1:A:435:C:H2'	1:A:436:C:H6	1.79	0.47
1:A:646:U:H2'	1:A:647:C:C6	2.48	0.47
1:A:715:A:H2'	1:A:716:A:C8	2.50	0.47
1:A:1197:G:H2'	1:A:1198:G:C5'	2.44	0.47
2:B:229:VAL:O	2:B:229:VAL:HG12	2.14	0.47
3:C:22:TRP:CG	3:C:59:ARG:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:GLU:O	3:C:59:ARG:HG3	2.13	0.47
3:C:123:GLN:O	3:C:128:PHE:HB2	2.14	0.47
3:C:157:ILE:HD12	3:C:164:ARG:CG	2.43	0.47
4:D:61:LYS:O	4:D:62:GLN:C	2.52	0.47
4:D:105:VAL:HG13	4:D:117:ALA:HB1	1.96	0.47
5:E:72:GLN:O	5:E:73:ASN:HB3	2.13	0.47
6:F:22:GLU:OE1	6:F:25:ILE:HD12	2.13	0.47
6:F:63:TYR:O	6:F:64:GLN:HB2	2.13	0.47
8:H:111:ILE:O	8:H:134:ILE:HB	2.14	0.47
9:I:40:LEU:C	9:I:42:ARG:N	2.68	0.47
10:J:5:ARG:HD2	10:J:99:LYS:CB	2.44	0.47
15:O:3:ILE:HG13	15:O:38:ARG:HH12	1.79	0.47
1:A:1186:G:N2	1:A:1187:G:H1'	2.29	0.47
1:A:1423:G:H2'	1:A:1424:C:H6	1.79	0.47
1:A:1481:U:H2'	1:A:1482:G:O4'	2.14	0.47
4:D:28:SER:O	4:D:29:PRO:C	2.52	0.47
6:F:4:TYR:CE2	6:F:72:VAL:HG22	2.49	0.47
8:H:100:ILE:CD1	8:H:112:LEU:HD11	2.44	0.47
8:H:122:ARG:HH11	8:H:122:ARG:HG3	1.79	0.47
10:J:8:LEU:CD1	10:J:70:ARG:HB2	2.39	0.47
12:L:54:LYS:N	12:L:54:LYS:CD	2.75	0.47
17:Q:90:ILE:O	17:Q:93:GLN:HB3	2.14	0.47
1:A:99:C:H2'	1:A:101:A:C1'	2.44	0.47
1:A:318:G:H2'	1:A:319:G:H8	1.79	0.47
1:A:420:U:O3'	1:A:421:U:H6	1.97	0.47
1:A:518:C:H4'	1:A:519:C:C6	2.44	0.47
1:A:691:G:H1'	1:A:696:A:N6	2.29	0.47
1:A:1402:C:O2	1:A:1500:A:N1	2.47	0.47
1:A:1461:G:O2'	1:A:1462:G:H5'	2.15	0.47
2:B:36:ARG:HB2	2:B:41:ILE:CD1	2.45	0.47
7:G:38:LEU:HD11	7:G:42:ILE:HD11	1.97	0.47
8:H:63:LEU:HD22	8:H:63:LEU:N	2.29	0.47
11:K:20:TYR:CD2	11:K:83:ILE:HB	2.49	0.47
14:N:35:ARG:O	14:N:37:PHE:N	2.48	0.47
19:S:27:GLU:HG3	19:S:47:HIS:CE1	2.49	0.47
19:S:47:HIS:O	19:S:62:ILE:HG22	2.15	0.47
1:A:83:U:O2'	1:A:84:U:H5'	2.14	0.47
1:A:142:G:N3	1:A:196:A:H2	2.13	0.47
1:A:252:U:H2'	1:A:253:U:C5	2.49	0.47
1:A:487:A:H2'	1:A:488:C:O4'	2.15	0.47
1:A:1058:G:O2'	1:A:1059:C:H5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1153:C:OP1	10:J:14:LYS:HD2	2.14	0.47
1:A:1202:G:H2'	1:A:1203:C:C5'	2.45	0.47
1:A:1407:C:H2'	1:A:1408:A:C8	2.46	0.47
2:B:49:GLU:H	2:B:49:GLU:CD	2.15	0.47
3:C:133:ALA:O	3:C:137:ALA:HB2	2.13	0.47
3:C:145:GLY:O	3:C:146:ALA:CB	2.63	0.47
4:D:158:ILE:HG22	4:D:181:MET:HE1	1.96	0.47
7:G:107:ALA:C	7:G:109:ASN:N	2.68	0.47
9:I:53:VAL:HG11	9:I:92:TYR:CZ	2.49	0.47
10:J:8:LEU:HD11	10:J:72:VAL:CG2	2.44	0.47
11:K:48:ILE:HD13	11:K:63:LEU:CB	2.45	0.47
12:L:54:LYS:O	12:L:70:ILE:HG13	2.14	0.47
12:L:59:ARG:CZ	12:L:65:GLU:HG2	2.45	0.47
14:N:35:ARG:C	14:N:37:PHE:N	2.67	0.47
21:V:9:ARG:CZ	21:V:23:PRO:HD2	2.44	0.47
1:A:60:A:H4'	1:A:61:G:O5'	2.14	0.47
1:A:164:U:H2'	1:A:165:C:H6	1.79	0.47
1:A:164:U:H2'	1:A:165:C:C6	2.49	0.47
1:A:491:G:H2'	1:A:492:G:C8	2.47	0.47
1:A:706:A:C5	1:A:707:C:C5	3.03	0.47
1:A:747:C:C5	1:A:748:C:C4	3.03	0.47
1:A:1031:G:H2'	1:A:1032:G:C8	2.49	0.47
1:A:1126:U:C5	1:A:1127:G:C6	3.03	0.47
1:A:1430:C:H2'	1:A:1431:C:C6	2.50	0.47
1:A:1447:G:H2'	1:A:1452:C:O5'	2.15	0.47
2:B:75:LYS:HB2	2:B:96:ARG:HH22	1.79	0.47
2:B:114:ARG:HH11	2:B:118:LEU:HD21	1.79	0.47
5:E:110:LEU:O	5:E:115:VAL:HB	2.15	0.47
6:F:94:GLN:O	6:F:95:GLU:C	2.52	0.47
7:G:64:GLN:NE2	7:G:68:ASN:HD21	2.12	0.47
9:I:66:ARG:HB3	9:I:66:ARG:NH1	2.30	0.47
11:K:34:ASP:C	11:K:34:ASP:OD2	2.52	0.47
12:L:36:VAL:H	12:L:58:VAL:HG13	1.79	0.47
12:L:53:ARG:N	12:L:53:ARG:HD2	2.30	0.47
12:L:92:ASP:HB3	12:L:93:LEU:CD2	2.44	0.47
13:M:4:ILE:HD11	13:M:56:LEU:CD1	2.45	0.47
13:M:37:THR:HG22	13:M:39:ILE:HG13	1.97	0.47
14:N:11:LYS:C	14:N:13:THR:H	2.18	0.47
15:O:16:ALA:CB	15:O:21:ASP:HB3	2.39	0.47
16:P:54:GLU:O	16:P:54:GLU:OE2	2.33	0.47
19:S:32:LYS:H	19:S:50:ALA:H	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:C:H2'	1:A:1162:C:C6	2.49	0.47
1:A:1347:G:H2'	1:A:1373:G:C6	2.49	0.47
2:B:44:LEU:O	2:B:47:THR:N	2.48	0.47
3:C:22:TRP:CZ2	3:C:32:LEU:O	2.67	0.47
5:E:34:VAL:HG12	5:E:62:ALA:HB1	1.96	0.47
8:H:29:SER:HB3	8:H:32:LYS:CG	2.42	0.47
15:O:53:HIS:HE1	15:O:57:LEU:HD11	1.79	0.47
1:A:186:C:H2'	1:A:187:C:C6	2.49	0.47
1:A:188:C:O3'	1:A:189:G:H4'	2.15	0.47
1:A:740:U:O3'	15:O:39:LEU:HD23	2.15	0.47
1:A:1328:C:OP1	21:V:21:TYR:OH	2.28	0.47
4:D:190:ASP:HB3	4:D:193:ASP:OD2	2.14	0.47
5:E:43:LEU:HB2	5:E:136:MET:CE	2.45	0.47
10:J:40:LEU:HD23	10:J:69:ASN:HB2	1.96	0.47
13:M:28:ALA:O	13:M:32:GLU:HB2	2.15	0.47
1:A:333:G:C4'	20:T:16:HIS:CD2	2.97	0.47
1:A:748:C:OP2	1:A:748:C:H6	1.98	0.47
1:A:942:G:H2'	1:A:943:U:C6	2.50	0.47
1:A:1032:G:H2'	1:A:1033:G:C8	2.49	0.47
1:A:1133:G:N1	1:A:1142:G:C6	2.83	0.47
1:A:1222:G:O2'	1:A:1223:C:H5'	2.14	0.47
1:A:1237:C:C4'	1:A:1334:G:H21	2.28	0.47
2:B:178:ARG:NH1	2:B:178:ARG:CG	2.68	0.47
4:D:19:LEU:O	4:D:20:TYR:O	2.33	0.47
7:G:10:ARG:HG2	7:G:10:ARG:HH11	1.79	0.47
7:G:72:ARG:HD3	7:G:142:GLU:OE1	2.14	0.47
10:J:24:VAL:HG11	10:J:34:VAL:HG11	1.97	0.47
13:M:86:CYS:SG	19:S:73:GLU:HG2	2.55	0.47
16:P:10:GLY:H	16:P:16:HIS:H	1.62	0.47
18:R:48:GLY:O	18:R:74:ARG:NH2	2.47	0.47
19:S:20:LEU:HD12	19:S:21:GLU:N	2.30	0.47
1:A:37:U:H2'	1:A:38:G:O4'	2.15	0.46
1:A:527:G:O2'	1:A:535:A:N1	2.42	0.46
1:A:620:C:C2	4:D:135:LEU:HD13	2.50	0.46
1:A:1057:G:C2'	1:A:1058:G:H5'	2.45	0.46
1:A:1176:A:H2'	1:A:1177:G:H8	1.79	0.46
1:A:1360:A:H2'	1:A:1361:G:O4'	2.15	0.46
6:F:18:GLN:CA	6:F:21:LEU:HB3	2.36	0.46
6:F:75:LEU:O	6:F:79:LEU:HB2	2.15	0.46
8:H:17:THR:C	8:H:78:GLN:HE22	2.18	0.46
9:I:70:LYS:HB3	9:I:70:LYS:NZ	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:5:ARG:HB3	10:J:99:LYS:O	2.15	0.46
13:M:79:LYS:O	13:M:82:MET:HB2	2.15	0.46
14:N:26:ARG:HD3	14:N:47:LEU:HD11	1.97	0.46
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.48	0.46
18:R:55:ARG:NH1	18:R:55:ARG:CB	2.77	0.46
19:S:27:GLU:HG3	19:S:47:HIS:ND1	2.30	0.46
19:S:28:LYS:HG2	19:S:29:ARG:H	1.79	0.46
1:A:1116:C:O2'	1:A:1117:G:H5'	2.14	0.46
1:A:1202:G:C2'	1:A:1203:C:H5'	2.46	0.46
2:B:68:ILE:H	2:B:90:MET:CE	2.12	0.46
3:C:83:ARG:O	3:C:85:ARG:N	2.39	0.46
3:C:118:GLN:O	3:C:121:ALA:HB3	2.16	0.46
4:D:59:ARG:NE	4:D:59:ARG:CA	2.74	0.46
8:H:31:PHE:HZ	8:H:134:ILE:HD13	1.80	0.46
9:I:4:TYR:HH	9:I:88:TYR:HD1	1.61	0.46
1:A:418:C:H2'	1:A:419:C:H6	1.81	0.46
1:A:419:C:H2'	1:A:420:U:O4'	2.16	0.46
1:A:492:G:H2'	1:A:494:G:C8	2.47	0.46
1:A:540:G:H2'	1:A:541:G:C8	2.50	0.46
1:A:1127:G:C2'	1:A:1128:C:H5'	2.45	0.46
1:A:1131:G:H2'	1:A:1132:C:C6	2.50	0.46
1:A:1392:G:H21	1:A:1502:A:H8	1.62	0.46
1:A:1414:U:H2'	1:A:1415:G:H8	1.80	0.46
2:B:68:ILE:HB	2:B:90:MET:CE	2.46	0.46
4:D:149:ALA:HB3	4:D:152:SER:OG	2.16	0.46
12:L:90:VAL:HG11	12:L:93:LEU:HD21	1.97	0.46
13:M:80:ARG:C	13:M:82:MET:H	2.17	0.46
13:M:103:THR:O	13:M:103:THR:HG22	2.15	0.46
15:O:85:LEU:HB3	15:O:87:ILE:HG13	1.98	0.46
1:A:392:G:H2'	1:A:393:A:H8	1.80	0.46
1:A:1124:G:H5"	10:J:35:SER:CA	2.45	0.46
2:B:13:ALA:HB1	2:B:17:PHE:CE2	2.50	0.46
3:C:78:GLY:O	3:C:79:ARG:HB3	2.15	0.46
3:C:84:ILE:O	3:C:84:ILE:HG23	2.15	0.46
4:D:47:ARG:HG2	4:D:48:ALA:N	2.30	0.46
4:D:190:ASP:O	4:D:193:ASP:N	2.48	0.46
5:E:107:ARG:CG	5:E:108:ALA:N	2.73	0.46
7:G:32:ARG:C	7:G:34:GLY:N	2.68	0.46
7:G:90:GLU:HG3	7:G:155:ARG:NH2	2.31	0.46
10:J:8:LEU:HD13	10:J:20:ALA:HB2	1.97	0.46
11:K:86:GLY:H	11:K:112:THR:HG23	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:4:ILE:HA	16:P:20:VAL:O	2.15	0.46
17:Q:29:HIS:HB2	17:Q:36:ILE:HD12	1.97	0.46
17:Q:29:HIS:CE1	17:Q:31:LEU:H	2.32	0.46
17:Q:40:LYS:HG2	17:Q:41:LYS:N	2.30	0.46
17:Q:45:HIS:HB3	17:Q:72:ARG:HG2	1.98	0.46
19:S:10:PHE:O	19:S:11:VAL:HG23	2.15	0.46
20:T:53:LEU:O	20:T:54:LYS:C	2.54	0.46
1:A:99:C:H2'	1:A:101:A:C8	2.50	0.46
1:A:135:C:O2	16:P:1:MET:HB2	2.15	0.46
1:A:191:G:C2'	1:A:192:U:O5'	2.63	0.46
1:A:443:C:O5'	1:A:443:C:H6	1.98	0.46
1:A:494:G:N2	1:A:495:U:O4	2.48	0.46
1:A:642:A:N7	8:H:115:SER:HA	2.30	0.46
1:A:783:C:O2'	1:A:784:C:H5'	2.15	0.46
1:A:971:G:OP1	1:A:971:G:H3'	2.15	0.46
1:A:976:G:H8	1:A:1358:U:H2'	1.80	0.46
1:A:1110:A:H8	1:A:1110:A:O5'	1.98	0.46
1:A:1121:U:H2'	1:A:1122:U:C6	2.51	0.46
1:A:1234:C:H4'	1:A:1364:U:H1'	1.98	0.46
1:A:1341:U:O2'	1:A:1342:C:H5'	2.16	0.46
2:B:42:ILE:CG2	2:B:43:ASP:N	2.79	0.46
3:C:44:GLU:HG2	3:C:52:LEU:HD22	1.96	0.46
7:G:148:ASN:C	7:G:150:ALA:N	2.68	0.46
9:I:33:PHE:C	9:I:35:GLU:H	2.18	0.46
19:S:41:VAL:HG22	19:S:44:MET:SD	2.56	0.46
19:S:77:THR:HG23	19:S:78:ARG:HG3	1.97	0.46
20:T:59:ALA:O	20:T:63:ILE:HG13	2.14	0.46
1:A:67:C:H4'	1:A:172:A:O4'	2.15	0.46
1:A:1251:A:H2'	1:A:1252:A:H8	1.81	0.46
2:B:53:ARG:NH1	2:B:199:TYR:CD2	2.83	0.46
2:B:91:PRO:HG3	2:B:154:LEU:CG	2.45	0.46
3:C:154:SER:O	3:C:155:GLY:O	2.32	0.46
3:C:155:GLY:C	3:C:196:LEU:HD22	2.35	0.46
6:F:23:LYS:O	6:F:27:GLN:HG2	2.15	0.46
9:I:64:THR:HG22	9:I:66:ARG:NH1	2.30	0.46
13:M:74:VAL:O	13:M:77:ASN:HB3	2.16	0.46
18:R:51:LEU:HD23	18:R:52:PRO:HD2	1.98	0.46
18:R:55:ARG:HH11	18:R:55:ARG:HA	1.81	0.46
19:S:41:VAL:HB	19:S:42:PRO:HD2	1.96	0.46
1:A:19:C:H2'	1:A:20:U:C6	2.48	0.46
1:A:52:G:O2'	1:A:53:A:H5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:C:H2'	1:A:132:C:H6	1.81	0.46
1:A:413:G:H2'	1:A:413:G:N3	2.30	0.46
1:A:605:U:O2'	1:A:606:G:H5'	2.16	0.46
1:A:616:G:O2'	1:A:617:G:H5'	2.15	0.46
1:A:1020:U:H2'	1:A:1021:G:H8	1.80	0.46
1:A:1267:C:O2	21:V:20:LYS:HD2	2.15	0.46
2:B:32:ILE:HG22	2:B:33:TYR:N	2.31	0.46
3:C:30:ARG:HG2	3:C:30:ARG:HH11	1.81	0.46
3:C:39:ILE:HG21	3:C:57:ILE:HD11	1.97	0.46
6:F:4:TYR:HD1	6:F:92:LYS:HA	1.80	0.46
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.97	0.46
9:I:114:TYR:CD1	10:J:59:SER:O	2.69	0.46
11:K:115:PRO:C	11:K:117:ASN:H	2.19	0.46
12:L:89:ARG:NH2	12:L:97:ARG:HH21	2.14	0.46
12:L:104:VAL:O	12:L:105:TYR:HB2	2.16	0.46
13:M:40:ASN:C	13:M:40:ASN:ND2	2.69	0.46
14:N:60:SER:O	14:N:61:TRP:HB3	2.16	0.46
19:S:73:GLU:HG2	19:S:73:GLU:O	2.16	0.46
1:A:147:G:C2	1:A:148:G:C8	3.03	0.46
1:A:317:G:O2'	1:A:318:G:H5'	2.16	0.46
1:A:502:G:C2	1:A:503:C:C2	3.03	0.46
1:A:577:G:H1'	1:A:816:A:C4	2.51	0.46
1:A:690:G:H2'	1:A:691:G:O4'	2.15	0.46
2:B:108:ILE:O	2:B:112:VAL:HG23	2.15	0.46
2:B:209:ARG:HE	2:B:239:VAL:CG1	2.29	0.46
4:D:205:GLU:O	4:D:206:PHE:C	2.54	0.46
6:F:53:ALA:O	6:F:54:LYS:CB	2.64	0.46
9:I:36:TYR:CD2	9:I:37:PHE:CE2	3.04	0.46
9:I:112:LYS:HD3	9:I:112:LYS:O	2.16	0.46
10:J:26:ALA:HB1	10:J:84:GLN:HE22	1.81	0.46
11:K:12:ARG:O	11:K:13:GLN:C	2.54	0.46
16:P:33:ILE:O	16:P:33:ILE:HG22	2.15	0.46
18:R:53:ARG:HG3	18:R:63:GLN:HB2	1.98	0.46
1:A:36:C:O2'	1:A:501:C:OP1	2.31	0.46
1:A:504:C:H41	12:L:115:LYS:HZ1	1.64	0.46
1:A:659:U:O2'	1:A:660:G:H5'	2.15	0.46
1:A:707:C:C2	1:A:708:C:C5	3.04	0.46
1:A:1233:G:H2'	1:A:1234:C:C6	2.51	0.46
1:A:1412:C:H2'	1:A:1413:A:C8	2.51	0.46
2:B:88:ALA:HB2	2:B:219:VAL:CG1	2.45	0.46
2:B:115:LEU:HD11	2:B:146:GLN:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:LEU:CB	2:B:142:LEU:HD21	2.46	0.46
3:C:164:ARG:NH1	3:C:166:GLU:OE1	2.49	0.46
17:Q:69:LYS:C	17:Q:70:ARG:HG3	2.36	0.46
17:Q:97:SER:O	17:Q:98:LEU:C	2.53	0.46
17:Q:104:LYS:HD3	17:Q:105:ALA:CB	2.46	0.46
1:A:671:G:H2'	1:A:672:U:C6	2.51	0.46
1:A:1100:C:O5'	1:A:1100:C:H6	1.99	0.46
1:A:1308:U:O2'	1:A:1309:G:H5'	2.16	0.46
1:A:1532:U:C2'	1:A:1533:C:H4'	2.46	0.46
2:B:107:THR:C	2:B:109:SER:N	2.69	0.46
3:C:5:ILE:CD1	3:C:10:PHE:HB2	2.45	0.46
5:E:128:PRO:O	5:E:130:ASN:N	2.48	0.46
6:F:42:GLU:HG3	6:F:61:LEU:HD23	1.98	0.46
6:F:101:ALA:HA	18:R:28:GLU:CB	2.46	0.46
7:G:15:ASP:OD2	7:G:16:LEU:N	2.49	0.46
9:I:118:LYS:NZ	9:I:118:LYS:HB3	2.30	0.46
11:K:124:LYS:HD3	11:K:125:PHE:CE1	2.51	0.46
1:A:691:G:O2'	1:A:797:C:H4'	2.16	0.45
1:A:922:G:H5'	5:E:19:MET:O	2.15	0.45
1:A:1293:G:O2'	1:A:1294:G:H5'	2.16	0.45
4:D:110:PHE:CD2	4:D:148:VAL:HG22	2.51	0.45
5:E:36:ASP:OD1	5:E:38:GLN:N	2.37	0.45
6:F:100:ASN:OD1	6:F:100:ASN:O	2.34	0.45
12:L:119:LYS:O	12:L:120:TYR:CB	2.64	0.45
13:M:96:LEU:C	13:M:110:ARG:HG2	2.37	0.45
14:N:11:LYS:C	14:N:13:THR:N	2.67	0.45
16:P:74:LEU:O	16:P:79:VAL:CG2	2.63	0.45
20:T:91:LEU:C	20:T:93:GLU:N	2.68	0.45
1:A:410:G:C2	1:A:429:U:C2	3.05	0.45
1:A:686:U:C2	1:A:687:A:N7	2.85	0.45
1:A:832:C:O2'	1:A:833:U:H5'	2.15	0.45
1:A:865:A:H2'	1:A:866:C:H6	1.81	0.45
1:A:1298:C:H2'	7:G:114:ARG:HH22	1.80	0.45
2:B:53:ARG:HG2	2:B:53:ARG:HH11	1.80	0.45
2:B:68:ILE:HD12	2:B:222:ILE:HD11	1.99	0.45
2:B:209:ARG:HE	2:B:239:VAL:HG13	1.82	0.45
3:C:81:GLY:HA2	3:C:84:ILE:CG2	2.46	0.45
3:C:101:LEU:O	3:C:101:LEU:CD2	2.65	0.45
3:C:167:TRP:O	3:C:168:ALA:CB	2.64	0.45
6:F:37:VAL:HG12	6:F:38:GLU:H	1.81	0.45
6:F:75:LEU:O	6:F:75:LEU:HD22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:34:ARG:HB3	12:L:61:THR:CG2	2.45	0.45
13:M:22:ILE:CG2	13:M:66:LEU:HD22	2.44	0.45
13:M:87:TYR:O	13:M:89:GLY:N	2.49	0.45
16:P:55:ARG:O	16:P:58:TYR:N	2.42	0.45
17:Q:27:PHE:O	17:Q:36:ILE:HD13	2.15	0.45
17:Q:104:LYS:HD3	17:Q:104:LYS:C	2.37	0.45
18:R:39:VAL:CG1	18:R:40:LEU:H	2.29	0.45
19:S:15:LEU:CA	19:S:18:LYS:HB3	2.32	0.45
19:S:63:THR:HG22	19:S:64:GLU:N	2.32	0.45
1:A:36:C:C4	1:A:37:U:C5	3.05	0.45
1:A:113:G:H2'	1:A:114:U:C6	2.52	0.45
1:A:166:G:H2'	1:A:167:G:H8	1.81	0.45
1:A:370:C:C2	1:A:371:G:C8	3.04	0.45
1:A:474:G:H5"	1:A:474:G:C2	2.50	0.45
1:A:513:C:O2'	1:A:514:C:H5'	2.16	0.45
1:A:710:G:H5"	6:F:54:LYS:HZ1	1.80	0.45
1:A:1015:A:H1'	1:A:1218:C:O2'	2.17	0.45
1:A:1347:G:O2'	1:A:1348:U:OP2	2.34	0.45
1:A:1406:U:H2'	1:A:1407:C:C5'	2.47	0.45
1:A:1423:G:H2'	1:A:1424:C:C6	2.52	0.45
2:B:194:PRO:C	2:B:196:LEU:H	2.20	0.45
3:C:107:GLN:H	3:C:107:GLN:CD	2.20	0.45
3:C:151:VAL:HG12	3:C:152:ILE:N	2.31	0.45
3:C:155:GLY:CA	3:C:196:LEU:HD22	2.46	0.45
4:D:76:ARG:CD	4:D:207:TYR:CE2	2.99	0.45
4:D:101:LEU:HD23	4:D:121:VAL:HG13	1.98	0.45
12:L:53:ARG:C	12:L:54:LYS:HD2	2.37	0.45
15:O:82:ILE:O	15:O:84:LYS:N	2.37	0.45
1:A:63:C:H6	1:A:63:C:H5'	1.81	0.45
1:A:147:G:O2'	1:A:148:G:H5'	2.17	0.45
1:A:1437:C:H2'	1:A:1438:G:C8	2.46	0.45
2:B:16:HIS:HD1	2:B:204:ASN:H	1.63	0.45
2:B:50:GLU:O	2:B:51:LEU:C	2.54	0.45
3:C:59:ARG:HG2	3:C:59:ARG:HH11	1.82	0.45
5:E:43:LEU:HB2	5:E:136:MET:HE2	1.96	0.45
7:G:75:VAL:CG1	7:G:76:ARG:H	2.27	0.45
7:G:79:ARG:HA	7:G:83:ALA:O	2.17	0.45
8:H:19:VAL:HG23	8:H:21:LYS:HG3	1.97	0.45
11:K:21:ILE:HD13	11:K:94:ALA:HB3	1.97	0.45
13:M:11:ARG:NH1	13:M:12:ASN:N	2.62	0.45
13:M:120:LYS:HE3	13:M:122:LYS:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:18:PHE:C	15:O:18:PHE:CD1	2.90	0.45
15:O:82:ILE:HD13	15:O:88:ARG:HG3	1.98	0.45
18:R:53:ARG:O	18:R:55:ARG:N	2.46	0.45
1:A:498:U:O2	1:A:498:U:H2'	2.16	0.45
1:A:529:G:H4'	1:A:533:A:C2	2.52	0.45
1:A:1262:C:H42	1:A:1273:G:H1	1.65	0.45
1:A:1305:G:H8	1:A:1305:G:OP2	2.00	0.45
4:D:29:PRO:O	4:D:30:LYS:HB2	2.17	0.45
5:E:5:ASP:O	5:E:6:PHE:O	2.35	0.45
7:G:5:ARG:HG2	7:G:6:ARG:N	2.31	0.45
9:I:108:VAL:CG1	9:I:109:VAL:H	2.20	0.45
9:I:110:GLU:HG2	9:I:113:LYS:HZ2	1.82	0.45
12:L:46:LYS:HE2	12:L:47:LYS:HG3	1.98	0.45
12:L:60:LEU:C	12:L:62:SER:H	2.20	0.45
12:L:83:VAL:HG21	12:L:100:ILE:HG21	1.99	0.45
19:S:23:ASN:C	19:S:25:LYS:N	2.70	0.45
19:S:28:LYS:C	19:S:29:ARG:HD2	2.37	0.45
19:S:32:LYS:CB	19:S:50:ALA:HB3	2.44	0.45
1:A:148:G:H2'	1:A:149:A:C8	2.49	0.45
1:A:321:A:O2'	1:A:322:C:H5'	2.17	0.45
1:A:381:C:H2'	1:A:382:A:C5'	2.47	0.45
1:A:760:G:C2'	1:A:761:G:H5'	2.46	0.45
1:A:762:C:H4'	17:Q:104:LYS:O	2.16	0.45
1:A:1521:G:H2'	1:A:1522:U:C6	2.52	0.45
3:C:75:VAL:HG12	3:C:75:VAL:O	2.16	0.45
3:C:114:PRO:O	3:C:118:GLN:HG3	2.16	0.45
7:G:47:CYS:HA	7:G:50:ILE:HG13	1.99	0.45
8:H:137:VAL:O	8:H:137:VAL:HG12	2.17	0.45
20:T:96:GLY:O	20:T:97:ALA:HB3	2.17	0.45
1:A:84:U:H2'	1:A:88:A:H8	1.82	0.45
1:A:188:C:O2	1:A:190:C:C4'	2.65	0.45
1:A:195:A:H4'	20:T:68:LYS:HD3	1.99	0.45
1:A:541:G:H2'	1:A:542:G:H8	1.81	0.45
1:A:1127:G:O2'	1:A:1128:C:H5'	2.17	0.45
1:A:1155:G:O2'	1:A:1156:G:H5'	2.16	0.45
1:A:1250:A:C4'	9:I:68:GLY:O	2.62	0.45
1:A:1518:A:C2	1:A:1519:A:C4	3.05	0.45
2:B:71:VAL:O	2:B:165:VAL:HG23	2.16	0.45
8:H:136:GLU:O	8:H:137:VAL:HG22	2.17	0.45
1:A:35:G:C2	12:L:118:SER:HB2	2.50	0.45
1:A:223:U:H2'	1:A:224:C:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:C:O2	1:A:371:G:C8	2.70	0.45
1:A:376:G:OP2	16:P:67:THR:HG21	2.17	0.45
1:A:613:C:O2	1:A:628:G:C2	2.70	0.45
1:A:1164:G:C6	1:A:1165:C:N4	2.85	0.45
1:A:1229:A:H2'	1:A:1230:C:C6	2.52	0.45
1:A:1250:A:H5"	9:I:68:GLY:H	1.81	0.45
1:A:1294:G:O2'	1:A:1295:G:H5'	2.17	0.45
1:A:1351:U:H4'	7:G:33:ASP:OD1	2.16	0.45
3:C:52:LEU:HD12	3:C:52:LEU:C	2.37	0.45
5:E:82:VAL:O	5:E:89:ILE:HG22	2.17	0.45
5:E:103:GLY:O	5:E:104:ALA:C	2.55	0.45
7:G:18:TYR:CD2	7:G:59:LEU:HD13	2.52	0.45
8:H:17:THR:HB	8:H:78:GLN:HE22	1.82	0.45
8:H:96:GLY:N	8:H:99:GLU:HB2	2.32	0.45
1:A:344:A:H5"	1:A:345:C:C5	2.52	0.45
1:A:397:A:C6	1:A:548:G:N7	2.85	0.45
1:A:401:C:O2'	1:A:402:G:H5'	2.17	0.45
1:A:791:G:C2'	1:A:792:A:C5'	2.94	0.45
2:B:97:TRP:O	2:B:98:LEU:O	2.35	0.45
2:B:130:ARG:HG3	2:B:134:GLU:OE1	2.17	0.45
5:E:84:PHE:O	5:E:87:SER:HB3	2.17	0.45
7:G:75:VAL:CG1	7:G:76:ARG:N	2.78	0.45
8:H:45:ILE:HD12	8:H:61:VAL:HG13	1.99	0.45
8:H:121:ASP:OD2	8:H:121:ASP:N	2.50	0.45
10:J:54:PHE:C	10:J:54:PHE:CD2	2.90	0.45
12:L:27:LEU:C	12:L:29:GLY:H	2.20	0.45
12:L:39:VAL:HG23	12:L:41:ARG:H	1.81	0.45
12:L:60:LEU:HD22	12:L:60:LEU:N	2.32	0.45
13:M:12:ASN:OD1	13:M:12:ASN:O	2.33	0.45
20:T:54:LYS:HG3	20:T:100:ILE:HD13	1.98	0.45
1:A:154:C:O5'	1:A:154:C:H6	2.00	0.45
1:A:278:G:OP2	17:Q:41:LYS:HE2	2.17	0.45
1:A:900:A:H2'	1:A:901:A:C8	2.52	0.45
1:A:976:G:C8	1:A:1358:U:H2'	2.52	0.45
1:A:1131:G:O2'	1:A:1132:C:H5'	2.17	0.45
1:A:1424:C:O2'	1:A:1425:U:H5'	2.17	0.45
1:A:1503:A:O5'	1:A:1531:A:H1'	2.17	0.45
3:C:16:ARG:HH21	3:C:54:ARG:HH21	1.65	0.45
4:D:3:ARG:O	4:D:4:TYR:HB3	2.16	0.45
11:K:101:SER:OG	11:K:102:GLY:N	2.49	0.45
12:L:101:VAL:HG12	12:L:104:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:3:ILE:N	15:O:3:ILE:CD1	2.79	0.45
20:T:74:LYS:HG3	20:T:75:ASN:H	1.81	0.45
1:A:16:A:C2	1:A:920:U:O2	2.70	0.44
1:A:406:G:H5'	4:D:5:ILE:HD13	1.98	0.44
1:A:474:G:H21	1:A:475:G:H1'	1.82	0.44
2:B:215:LEU:O	2:B:219:VAL:HG23	2.17	0.44
3:C:94:LEU:O	3:C:94:LEU:HD23	2.17	0.44
3:C:116:VAL:HG11	3:C:141:VAL:HG21	1.99	0.44
4:D:162:LEU:HA	4:D:165:MET:HG2	1.99	0.44
5:E:80:ILE:HD12	5:E:91:LEU:HD12	1.99	0.44
7:G:54:THR:HG22	7:G:55:GLY:N	2.30	0.44
7:G:93:PRO:O	7:G:96:GLN:HB3	2.17	0.44
8:H:80:ILE:O	8:H:80:ILE:HG22	2.17	0.44
8:H:126:LYS:C	8:H:128:GLY:H	2.21	0.44
11:K:109:VAL:CG1	18:R:84:LYS:HB3	2.47	0.44
14:N:14:PRO:O	14:N:15:LYS:HB2	2.17	0.44
14:N:26:ARG:HD2	14:N:47:LEU:HD21	1.99	0.44
1:A:532:A:C5	3:C:161:GLU:HB2	2.52	0.44
1:A:603:U:H2'	1:A:604:G:C8	2.52	0.44
1:A:890:G:O2'	1:A:906:G:O6	2.28	0.44
1:A:966:G:O2'	1:A:967:C:H5'	2.16	0.44
1:A:1205:U:HO2'	1:A:1206:G:H8	1.64	0.44
3:C:70:VAL:O	3:C:106:VAL:N	2.50	0.44
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.99	0.44
7:G:104:LEU:HD23	7:G:104:LEU:HA	1.84	0.44
17:Q:4:LYS:HE3	17:Q:6:LEU:HD21	1.98	0.44
18:R:55:ARG:HH11	18:R:55:ARG:CB	2.30	0.44
20:T:73:HIS:O	20:T:76:ALA:HB3	2.17	0.44
1:A:55:A:C2	1:A:56:U:C1'	3.00	0.44
1:A:104:G:O6	20:T:14:LYS:NZ	2.51	0.44
1:A:191:G:C8	1:A:191:G:C4'	3.00	0.44
1:A:247:G:C6	1:A:278:G:C2	3.05	0.44
1:A:335:C:H2'	1:A:336:C:C6	2.53	0.44
1:A:390:C:H2'	1:A:391:G:C8	2.52	0.44
1:A:969:A:O2'	1:A:970:C:H5'	2.17	0.44
1:A:1006:A:H5'	1:A:1006(A):C:C4'	2.45	0.44
1:A:1072:G:H1	1:A:1103:C:N4	2.15	0.44
1:A:1402:C:C5	1:A:1403:C:C5	3.06	0.44
3:C:34:LEU:HD22	3:C:38:ARG:HG3	1.98	0.44
4:D:11:LEU:O	4:D:15:GLU:HB2	2.17	0.44
5:E:18:ARG:HE	5:E:25:ARG:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:4:TYR:CE2	6:F:72:VAL:CG2	3.00	0.44
7:G:21:VAL:O	7:G:23:VAL:N	2.50	0.44
11:K:25:TYR:OH	11:K:87:THR:HB	2.18	0.44
16:P:9:PHE:O	16:P:10:GLY:O	2.36	0.44
19:S:11:VAL:HG22	19:S:39:THR:N	2.33	0.44
1:A:35:G:H2'	1:A:36:C:H6	1.79	0.44
1:A:173:U:H6	1:A:198:G:HO2'	1.56	0.44
1:A:187:C:O2'	20:T:89:ARG:NE	2.42	0.44
1:A:188:C:O2	1:A:190:C:H4'	2.17	0.44
1:A:375:U:OP1	16:P:69:THR:HG21	2.17	0.44
1:A:559:A:H4'	1:A:560:U:O3'	2.17	0.44
1:A:1021:G:O2'	1:A:1022:G:H5'	2.18	0.44
1:A:1034:G:H2'	1:A:1035:A:H8	1.83	0.44
1:A:1215:G:H2'	1:A:1215:G:N3	2.33	0.44
1:A:1257:U:O2'	1:A:1258:G:OP2	2.27	0.44
2:B:30:ARG:HD2	2:B:31:TYR:CZ	2.52	0.44
2:B:77:ALA:HB2	2:B:208:ILE:HG12	1.98	0.44
3:C:134:ILE:HG22	3:C:168:ALA:HB2	1.98	0.44
3:C:155:GLY:O	3:C:196:LEU:HD22	2.18	0.44
6:F:91:VAL:HG21	18:R:72:ARG:NH1	2.32	0.44
7:G:116:ALA:O	7:G:120:ILE:HG13	2.17	0.44
7:G:129:GLU:OE1	7:G:131:LYS:HE2	2.17	0.44
7:G:138:LYS:C	7:G:138:LYS:HD3	2.37	0.44
12:L:83:VAL:CG2	12:L:100:ILE:HG23	2.48	0.44
18:R:55:ARG:HB3	18:R:55:ARG:CZ	2.46	0.44
19:S:15:LEU:O	19:S:19:VAL:N	2.50	0.44
20:T:55:ILE:O	20:T:58:LYS:N	2.50	0.44
1:A:47:C:H5"	1:A:365:U:C6	2.51	0.44
1:A:62:U:C2'	1:A:63:C:C5'	2.93	0.44
1:A:188:C:C4	1:A:189:G:N3	2.86	0.44
1:A:340:U:H2'	1:A:341:C:C6	2.53	0.44
1:A:828:A:N6	1:A:858:G:O2'	2.45	0.44
1:A:1026:G:O6	1:A:1035:A:N1	2.50	0.44
1:A:1286:A:H2	21:V:18:TYR:HH	1.61	0.44
2:B:81:VAL:HG12	2:B:92:TYR:CD1	2.46	0.44
2:B:118:LEU:C	2:B:120:ALA:N	2.70	0.44
3:C:131:ARG:HH21	3:C:164:ARG:CZ	2.30	0.44
3:C:175:LEU:HD11	3:C:201:TYR:CE2	2.53	0.44
4:D:96:LEU:N	4:D:96:LEU:CD1	2.81	0.44
8:H:31:PHE:CE1	8:H:35:ILE:HD11	2.52	0.44
9:I:27:THR:HG22	9:I:28:VAL:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:14:VAL:O	11:K:15:ALA:CB	2.65	0.44
15:O:17:ARG:NH2	15:O:77:ARG:HD3	2.32	0.44
18:R:62:GLU:C	18:R:64:ARG:N	2.68	0.44
19:S:51:VAL:HB	19:S:75:ALA:HB2	2.00	0.44
1:A:55:A:O2'	1:A:56:U:H5'	2.18	0.44
1:A:1040:U:H2'	1:A:1041:A:H8	1.82	0.44
1:A:1145:C:O2'	1:A:1146:A:P	2.76	0.44
1:A:1287:A:C6	1:A:1288:A:C6	3.06	0.44
1:A:1327:C:H5"	21:V:20:LYS:CB	2.47	0.44
1:A:1415:G:C4	1:A:1416:G:C8	3.06	0.44
2:B:8:LYS:O	2:B:9:GLU:CB	2.64	0.44
3:C:58:GLU:CG	10:J:92:THR:HG21	2.48	0.44
6:F:67:MET:HE1	6:F:72:VAL:HA	2.00	0.44
9:I:50:LEU:C	9:I:52:ALA:H	2.21	0.44
10:J:40:LEU:CG	10:J:41:PRO:HD2	2.47	0.44
12:L:117:ARG:C	12:L:119:LYS:N	2.70	0.44
20:T:13:LEU:H	20:T:13:LEU:CD1	2.29	0.44
23:Y:35:C:C5	23:Y:36:C:H5	2.35	0.44
1:A:389:A:H2'	1:A:390:C:O4'	2.18	0.44
1:A:858:G:O2'	1:A:859:A:H5'	2.18	0.44
1:A:877:C:O2	8:H:3:THR:CG2	2.58	0.44
1:A:1213:A:C6	1:A:1215:G:H1'	2.52	0.44
1:A:1367:C:P	9:I:112:LYS:HZ1	2.41	0.44
2:B:103:THR:HB	2:B:176:GLU:OE1	2.18	0.44
2:B:115:LEU:O	2:B:115:LEU:HG	2.17	0.44
3:C:124:ILE:O	3:C:124:ILE:HG22	2.18	0.44
3:C:173:VAL:N	3:C:174:PRO:CD	2.80	0.44
4:D:59:ARG:HA	4:D:59:ARG:HE	1.81	0.44
4:D:105:VAL:HG13	4:D:105:VAL:O	2.17	0.44
4:D:118:ARG:NH2	4:D:118:ARG:HG3	2.32	0.44
9:I:109:VAL:O	9:I:109:VAL:HG12	2.17	0.44
13:M:108:ARG:NE	13:M:108:ARG:HA	2.32	0.44
14:N:29:ARG:HD3	14:N:40:CYS:HB2	2.00	0.44
1:A:839:U:O2	1:A:839:U:C2'	2.65	0.44
1:A:1104:G:H2'	1:A:1105:A:H8	1.82	0.44
1:A:1286:A:H4'	21:V:25:LYS:NZ	2.32	0.44
2:B:53:ARG:NH1	2:B:199:TYR:HD2	2.16	0.44
2:B:177:ALA:HB1	2:B:182:ILE:O	2.17	0.44
4:D:56:VAL:O	4:D:58:LEU:N	2.51	0.44
4:D:62:GLN:HE22	4:D:65:ARG:HH11	1.65	0.44
7:G:60:LYS:O	7:G:63:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:115:LYS:HB3	12:L:116:SER:H	1.61	0.44
13:M:4:ILE:HD13	13:M:19:LEU:HD21	1.99	0.44
18:R:43:PHE:HA	18:R:51:LEU:HD12	2.00	0.44
19:S:63:THR:HG22	19:S:64:GLU:H	1.82	0.44
1:A:9:G:C5'	5:E:122:GLU:OE2	2.60	0.44
1:A:21:G:N2	1:A:22:G:C6	2.86	0.44
1:A:35:G:N2	12:L:118:SER:HB2	2.33	0.44
1:A:381:C:C2'	1:A:382:A:H5'	2.48	0.44
1:A:625:G:O2'	1:A:626:U:H5'	2.17	0.44
1:A:865:A:O2'	1:A:866:C:H5'	2.18	0.44
1:A:1190:G:C2'	1:A:1191:A:OP2	2.66	0.44
1:A:1243:C:H2'	1:A:1244:C:C6	2.53	0.44
1:A:1379:G:C6	1:A:1380:U:C4	3.05	0.44
1:A:1481:U:C2'	1:A:1482:G:H5'	2.48	0.44
3:C:22:TRP:HA	10:J:93:GLY:HA2	1.98	0.44
3:C:103:VAL:HG12	3:C:104:GLN:N	2.32	0.44
3:C:191:THR:HG22	3:C:193:TYR:H	1.82	0.44
4:D:3:ARG:HG3	4:D:118:ARG:HE	1.83	0.44
5:E:10:MET:CE	5:E:10:MET:H	2.31	0.44
5:E:110:LEU:HD13	5:E:118:ILE:HD13	2.00	0.44
11:K:24:SER:C	11:K:26:ASN:H	2.21	0.44
12:L:6:THR:HG1	12:L:9:GLN:HG3	1.77	0.44
15:O:18:PHE:HD1	15:O:19:PRO:O	2.01	0.44
15:O:57:LEU:HD12	15:O:57:LEU:N	2.32	0.44
16:P:20:VAL:HG13	16:P:32:TYR:HB2	2.00	0.44
20:T:41:VAL:O	20:T:42:GLN:C	2.55	0.44
21:V:9:ARG:NH2	21:V:23:PRO:HD2	2.33	0.44
1:A:126:G:H5'	1:A:633:G:N2	2.33	0.43
1:A:426:G:H2'	1:A:427:U:C6	2.53	0.43
1:A:925:G:C2	1:A:927:G:C8	3.05	0.43
1:A:1006:A:O5'	1:A:1006(A):C:H5"	2.17	0.43
1:A:1030(A):G:H22	1:A:1030(C):G:H3'	1.83	0.43
1:A:1123:A:C2	10:J:39:PRO:HG3	2.51	0.43
1:A:1134:G:H1	1:A:1140:C:N4	2.16	0.43
1:A:1372:U:H5"	9:I:71:SER:HB3	2.00	0.43
1:A:1518:A:N1	1:A:1519:A:C6	2.86	0.43
2:B:60:ASP:O	2:B:64:ARG:HB2	2.17	0.43
11:K:58:PRO:HB2	11:K:93:GLN:HG3	1.99	0.43
12:L:57:LYS:HD3	12:L:67:THR:HB	1.98	0.43
13:M:80:ARG:O	13:M:84:ILE:HG23	2.17	0.43
1:A:16:A:O2'	1:A:17:U:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:G:O2'	1:A:168:G:H5'	2.17	0.43
1:A:460:A:O2'	1:A:461:C:H5"	2.18	0.43
1:A:939:G:H2'	1:A:940:C:H6	1.83	0.43
1:A:952:U:O2'	1:A:953:G:H5'	2.17	0.43
2:B:8:LYS:H	2:B:217:ARG:HH12	1.66	0.43
2:B:140:HIS:O	2:B:143:GLU:HB2	2.18	0.43
3:C:129:ALA:CB	3:C:132:ARG:HB2	2.48	0.43
3:C:188:LEU:HD11	3:C:195:VAL:HG13	2.00	0.43
4:D:8:VAL:HG22	4:D:115:ARG:NH2	2.33	0.43
4:D:196:LEU:C	4:D:198:VAL:H	2.22	0.43
5:E:15:ARG:HD2	5:E:15:ARG:C	2.38	0.43
5:E:18:ARG:HG2	5:E:19:MET:N	2.33	0.43
6:F:81:ILE:O	6:F:81:ILE:HG22	2.18	0.43
10:J:92:THR:HG22	10:J:93:GLY:N	2.32	0.43
11:K:72:ALA:O	11:K:77:MET:HB2	2.18	0.43
11:K:84:VAL:O	11:K:85:ARG:HG3	2.18	0.43
15:O:43:LEU:HD11	15:O:53:HIS:HA	2.00	0.43
20:T:83:ARG:HA	20:T:86:ARG:HD3	2.00	0.43
1:A:17:U:H2'	1:A:18:C:C6	2.54	0.43
1:A:315:A:O4'	1:A:353:A:C2	2.71	0.43
1:A:393:A:OP2	16:P:12:LYS:NZ	2.44	0.43
1:A:836:G:C6	1:A:851:G:C6	3.06	0.43
1:A:997:U:O2'	1:A:998:G:H5'	2.17	0.43
1:A:1006:A:OP1	1:A:1038:C:C4'	2.64	0.43
1:A:1193:G:C2	1:A:1194:U:C6	3.06	0.43
1:A:1346:A:C8	7:G:10:ARG:NH2	2.86	0.43
3:C:74:GLY:C	3:C:76:VAL:N	2.69	0.43
5:E:78:HIS:C	5:E:78:HIS:ND1	2.72	0.43
6:F:36:ARG:O	6:F:65:VAL:HA	2.18	0.43
9:I:100:GLY:C	9:I:102:LEU:N	2.71	0.43
10:J:7:LYS:CE	10:J:99:LYS:HZ1	2.31	0.43
11:K:14:VAL:HG21	11:K:40:ILE:HD13	1.97	0.43
13:M:4:ILE:CD1	13:M:56:LEU:HD13	2.49	0.43
17:Q:33:GLY:O	17:Q:34:LYS:C	2.55	0.43
17:Q:101:ARG:HA	17:Q:101:ARG:NE	2.33	0.43
1:A:103:C:OP1	20:T:17:ARG:NH1	2.50	0.43
1:A:895:G:H2'	1:A:896:C:H6	1.81	0.43
1:A:1040:U:H2'	1:A:1041:A:C8	2.53	0.43
1:A:1160:G:H4'	2:B:132:LYS:NZ	2.34	0.43
2:B:121:LEU:HD22	2:B:122:PHE:CE1	2.53	0.43
5:E:74:GLY:HA3	5:E:116:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.32	0.43
7:G:98:SER:C	7:G:100:ALA:N	2.70	0.43
13:M:123:ALA:HA	13:M:124:PRO:HD3	1.85	0.43
14:N:43:CYS:O	14:N:47:LEU:HG	2.19	0.43
18:R:33:ASP:OD2	18:R:36:ASN:HB2	2.18	0.43
19:S:31:ILE:O	19:S:32:LYS:O	2.37	0.43
1:A:107:G:H2'	1:A:108:G:C5'	2.45	0.43
1:A:650:G:O2'	1:A:651:C:H5'	2.18	0.43
1:A:737:A:OP1	6:F:92:LYS:HG3	2.18	0.43
1:A:1307:U:H2'	1:A:1308:U:C6	2.54	0.43
1:A:1315:U:OP2	19:S:6:LYS:NZ	2.44	0.43
1:A:1356:G:C2'	1:A:1357:A:H8	2.19	0.43
1:A:1371:G:H2'	1:A:1372:U:H6	1.82	0.43
1:A:1399:C:C2	1:A:1401:G:C5	3.06	0.43
2:B:28:PHE:O	2:B:32:ILE:HG13	2.18	0.43
4:D:67:ILE:HG22	4:D:68:TYR:N	2.32	0.43
4:D:118:ARG:HG3	4:D:118:ARG:HH21	1.83	0.43
4:D:162:LEU:HD13	4:D:181:MET:HE3	2.01	0.43
5:E:31:LEU:HD11	5:E:43:LEU:HD21	1.98	0.43
7:G:12:LEU:HD12	7:G:12:LEU:N	2.25	0.43
7:G:47:CYS:HA	7:G:50:ILE:CG1	2.49	0.43
11:K:30:VAL:HG21	11:K:65:ALA:HA	2.00	0.43
13:M:9:ILE:N	13:M:9:ILE:CD1	2.76	0.43
16:P:6:LEU:HB3	16:P:17:TYR:CD2	2.52	0.43
16:P:67:THR:HB	16:P:70:ALA:CB	2.48	0.43
1:A:230:G:H2'	1:A:231:G:O4'	2.19	0.43
1:A:458:C:N3	1:A:474:G:N1	2.63	0.43
1:A:737:A:H2'	1:A:738:C:H6	1.82	0.43
1:A:1028:C:H2'	1:A:1029:C:O4'	2.19	0.43
1:A:1205:U:H4'	3:C:195:VAL:CG2	2.48	0.43
1:A:1320:C:N3	19:S:36:ARG:NH1	2.67	0.43
1:A:1513:A:H2'	1:A:1514:C:C6	2.54	0.43
3:C:64:VAL:CG2	3:C:99:VAL:HG11	2.47	0.43
4:D:59:ARG:O	4:D:62:GLN:HB2	2.19	0.43
6:F:2:ARG:NH2	15:O:2:PRO:HD3	2.34	0.43
6:F:42:GLU:HG3	6:F:61:LEU:CD2	2.48	0.43
8:H:41:ARG:HG2	8:H:41:ARG:NH1	2.34	0.43
8:H:123:GLU:O	8:H:126:LYS:HB3	2.19	0.43
9:I:28:VAL:HG21	9:I:33:PHE:CD1	2.52	0.43
10:J:17:ASP:O	10:J:21:GLN:HB2	2.19	0.43
10:J:48:THR:HG1	10:J:62:HIS:CD2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:34:ASP:O	11:K:36:ASP:N	2.52	0.43
17:Q:76:LEU:HD23	17:Q:78:GLU:N	2.33	0.43
1:A:21:G:C2	1:A:22:G:C6	3.07	0.43
1:A:105:G:H2'	1:A:106:C:H6	1.82	0.43
1:A:192:U:O2'	20:T:57:ARG:HG3	2.19	0.43
1:A:436:C:H5"	4:D:156:GLU:CD	2.38	0.43
1:A:451:A:C5	1:A:481:G:C6	3.07	0.43
1:A:502:G:H2'	1:A:503:C:C6	2.53	0.43
1:A:1104:G:H4'	2:B:111:ARG:CZ	2.49	0.43
1:A:1345:U:C4	1:A:1377:A:N3	2.86	0.43
1:A:1346:A:C8	1:A:1348:U:C2	3.07	0.43
2:B:48:MET:O	2:B:51:LEU:HB2	2.17	0.43
2:B:55:PHE:O	2:B:56:ARG:C	2.57	0.43
7:G:142:GLU:O	7:G:145:ALA:HB3	2.17	0.43
8:H:31:PHE:HZ	8:H:134:ILE:CD1	2.32	0.43
9:I:13:ALA:HA	9:I:67:GLY:O	2.18	0.43
10:J:35:SER:O	10:J:36:GLY:O	2.36	0.43
11:K:30:VAL:HG12	11:K:31:THR:N	2.32	0.43
11:K:46:GLY:O	11:K:47:VAL:C	2.57	0.43
12:L:55:VAL:O	12:L:56:ALA:HB2	2.17	0.43
12:L:110:VAL:HG21	12:L:120:TYR:HB3	2.01	0.43
17:Q:100:LYS:O	17:Q:101:ARG:HB2	2.17	0.43
18:R:16:PRO:HG2	18:R:17:SER:H	1.83	0.43
1:A:410:G:H2'	1:A:429:U:C5	2.53	0.43
1:A:642:A:C8	8:H:115:SER:HA	2.53	0.43
1:A:644:G:O2'	1:A:645:C:H5'	2.19	0.43
1:A:1132:C:H2'	1:A:1133:G:H8	1.83	0.43
1:A:1365:G:C2'	1:A:1366:C:H5'	2.49	0.43
2:B:16:HIS:HB3	2:B:17:PHE:H	1.37	0.43
2:B:30:ARG:HG3	2:B:31:TYR:CD2	2.54	0.43
3:C:77:ILE:O	3:C:83:ARG:N	2.51	0.43
3:C:83:ARG:HA	3:C:86:VAL:HG23	2.01	0.43
7:G:59:LEU:O	7:G:60:LYS:C	2.57	0.43
8:H:39:LEU:HD12	8:H:44:PHE:HD2	1.84	0.43
8:H:126:LYS:C	8:H:128:GLY:N	2.72	0.43
19:S:77:THR:CG2	19:S:78:ARG:N	2.81	0.43
20:T:53:LEU:CD1	20:T:101:GLY:H	2.32	0.43
20:T:94:ALA:O	20:T:95:ALA:HB3	2.18	0.43
1:A:148:G:C2	1:A:149:A:C5	3.06	0.43
1:A:544:G:OP1	4:D:62:GLN:OE1	2.37	0.43
1:A:586:C:O3'	8:H:89:PRO:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:U:OP1	16:P:35:LYS:NZ	2.50	0.43
1:A:849:C:O2'	1:A:850:U:H5'	2.19	0.43
1:A:858:G:O6	1:A:869:G:H3'	2.19	0.43
1:A:867:G:O2'	1:A:868:C:H5'	2.19	0.43
1:A:1004:A:N7	1:A:1026:G:C5	2.86	0.43
1:A:1186:G:C2	1:A:1187:G:C8	3.06	0.43
1:A:1187:G:O2'	9:I:111:ARG:NH1	2.51	0.43
1:A:1368:G:OP2	9:I:112:LYS:CD	2.57	0.43
1:A:1478:C:H2'	1:A:1479:C:C6	2.54	0.43
2:B:44:LEU:C	2:B:46:LYS:N	2.72	0.43
2:B:51:LEU:HD22	2:B:55:PHE:CE1	2.53	0.43
2:B:90:MET:HA	2:B:91:PRO:HD3	1.93	0.43
2:B:140:HIS:ND1	2:B:143:GLU:HG3	2.34	0.43
2:B:170:GLU:HG3	2:B:170:GLU:O	2.18	0.43
3:C:64:VAL:CG1	3:C:65:ALA:N	2.81	0.43
3:C:173:VAL:O	3:C:173:VAL:HG12	2.19	0.43
4:D:41:GLY:C	4:D:43:HIS:H	2.20	0.43
4:D:190:ASP:O	4:D:194:LEU:HD22	2.19	0.43
6:F:101:ALA:HA	18:R:28:GLU:CG	2.49	0.43
7:G:28:ASN:OD1	7:G:36:LYS:NZ	2.51	0.43
8:H:112:LEU:N	8:H:112:LEU:CD2	2.81	0.43
9:I:99:LEU:HB3	9:I:101:PHE:CD1	2.53	0.43
18:R:70:ILE:HG22	18:R:71:LYS:N	2.32	0.43
18:R:88:LYS:OXT	18:R:88:LYS:HG2	2.19	0.43
19:S:15:LEU:O	19:S:19:VAL:HG12	2.19	0.43
1:A:81:U:O2'	1:A:82:U:P	2.76	0.43
1:A:521:G:OP2	12:L:54:LYS:HE2	2.19	0.43
1:A:528:C:H5'	1:A:535:A:N6	2.33	0.43
1:A:959:A:C2'	1:A:960:U:H4'	2.49	0.43
1:A:994:A:N7	1:A:1216:G:C4'	2.82	0.43
1:A:1030(D):A:H8	1:A:1030(D):A:O5'	2.01	0.43
1:A:1118:C:H5'	9:I:104:ARG:HG3	2.01	0.43
1:A:1508:G:C5	1:A:1509:C:C5	3.06	0.43
2:B:16:HIS:NE2	2:B:214:ILE:HG12	2.34	0.43
4:D:10:ARG:NH1	4:D:40:PRO:HG3	2.34	0.43
4:D:18:LYS:HD3	4:D:20:TYR:CE2	2.37	0.43
4:D:175:SER:HB3	4:D:186:LEU:HD11	2.00	0.43
9:I:12:GLU:HG2	9:I:12:GLU:O	2.19	0.43
10:J:12:ASP:OD1	10:J:15:THR:N	2.50	0.43
15:O:71:GLN:O	15:O:71:GLN:HG2	2.17	0.43
17:Q:49:GLU:O	17:Q:50:LYS:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:11:SER:HA	20:T:13:LEU:HD13	2.00	0.43
1:A:9:G:OP2	5:E:121:LYS:NZ	2.38	0.42
1:A:180:U:C2'	1:A:181:G:H5'	2.45	0.42
1:A:333:G:H4'	20:T:16:HIS:HE2	1.84	0.42
1:A:364:A:H2'	1:A:365:U:O2	2.19	0.42
1:A:648:A:O2'	1:A:649:G:H5'	2.19	0.42
1:A:807:A:H2'	1:A:808:C:C6	2.54	0.42
1:A:1101:A:H4'	1:A:1102:A:O5'	2.18	0.42
1:A:1281:U:H5'	1:A:1282:C:C5	2.49	0.42
1:A:1320:C:OP1	19:S:70:LYS:NZ	2.51	0.42
1:A:1346:A:C5	7:G:10:ARG:NH2	2.87	0.42
2:B:17:PHE:HD2	2:B:44:LEU:HD11	1.83	0.42
2:B:53:ARG:NH1	2:B:53:ARG:HG2	2.34	0.42
3:C:105:GLU:O	3:C:107:GLN:NE2	2.53	0.42
3:C:107:GLN:O	3:C:108:ASN:HB2	2.17	0.42
5:E:74:GLY:CA	5:E:116:THR:HG22	2.47	0.42
5:E:151:LEU:HD11	8:H:77:GLU:OE2	2.18	0.42
8:H:120:THR:HG23	8:H:123:GLU:CD	2.39	0.42
9:I:56:LEU:HD23	9:I:56:LEU:C	2.38	0.42
9:I:60:ASP:O	9:I:61:ALA:CB	2.67	0.42
10:J:4:ILE:HA	10:J:100:THR:CB	2.49	0.42
10:J:9:ARG:HG2	10:J:9:ARG:NH1	2.34	0.42
12:L:46:LYS:CE	12:L:47:LYS:HE3	2.48	0.42
12:L:93:LEU:CG	12:L:96:VAL:HG21	2.49	0.42
15:O:4:THR:OG1	15:O:7:GLU:HG3	2.19	0.42
16:P:18:ARG:NH1	16:P:32:TYR:OH	2.51	0.42
17:Q:11:VAL:HA	17:Q:53:LEU:HD11	2.00	0.42
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.83	0.42
1:A:17:U:O2'	1:A:1079:G:H1'	2.19	0.42
1:A:492:G:O2'	1:A:494:G:H5'	2.19	0.42
1:A:723:U:O2	1:A:723:U:C2'	2.65	0.42
1:A:789:U:O2'	1:A:791:G:N7	2.46	0.42
1:A:839:U:O2	1:A:839:U:H2'	2.19	0.42
1:A:958:A:N3	1:A:985:C:O2'	2.46	0.42
1:A:972:C:OP1	10:J:57:LYS:HE2	2.20	0.42
1:A:989:C:N4	1:A:1216:G:H1	2.17	0.42
1:A:1123:A:H4'	10:J:37:PRO:CD	2.28	0.42
1:A:1216:G:O3'	14:N:5:ALA:HB1	2.19	0.42
1:A:1321:C:H2'	1:A:1322:C:C5	2.54	0.42
1:A:1354:C:H2'	1:A:1355:G:H8	1.83	0.42
2:B:139:LYS:HD3	2:B:139:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:ARG:HG2	3:C:63:ASN:O	2.20	0.42
4:D:11:LEU:HD13	4:D:66:ARG:HB3	2.01	0.42
4:D:58:LEU:O	4:D:59:ARG:C	2.58	0.42
4:D:68:TYR:N	4:D:68:TYR:CD1	2.87	0.42
5:E:6:PHE:HZ	5:E:66:MET:HE1	1.83	0.42
5:E:103:GLY:C	5:E:106:PRO:HD2	2.39	0.42
9:I:113:LYS:H	9:I:113:LYS:CD	2.31	0.42
11:K:84:VAL:CG1	11:K:85:ARG:N	2.82	0.42
13:M:67:GLU:O	13:M:68:GLY:C	2.57	0.42
18:R:24:ALA:O	18:R:26:LEU:N	2.46	0.42
19:S:41:VAL:HG23	19:S:44:MET:HG3	2.00	0.42
1:A:324:G:H5"	1:A:324:G:H8	1.84	0.42
1:A:452:A:O3'	16:P:72:ARG:HD2	2.19	0.42
1:A:678:U:H4'	1:A:778:G:OP1	2.19	0.42
1:A:909:A:OP1	12:L:21:LYS:HD3	2.18	0.42
1:A:1096:C:H2'	1:A:1097:C:C6	2.52	0.42
1:A:1443:G:H5"	1:A:1446:A:C5'	2.47	0.42
2:B:194:PRO:C	2:B:196:LEU:N	2.71	0.42
3:C:34:LEU:CD2	3:C:38:ARG:HG3	2.50	0.42
3:C:179:ARG:O	3:C:179:ARG:CG	2.67	0.42
4:D:52:SER:O	4:D:53:ASP:C	2.58	0.42
4:D:150:GLU:O	4:D:152:SER:N	2.51	0.42
7:G:107:ALA:O	7:G:109:ASN:N	2.52	0.42
9:I:65:VAL:HG22	9:I:73:GLN:HB3	2.00	0.42
13:M:34:LEU:CD1	13:M:41:PRO:HA	2.49	0.42
15:O:26:GLU:N	15:O:26:GLU:OE2	2.52	0.42
20:T:11:SER:CA	20:T:13:LEU:HD13	2.50	0.42
1:A:194:C:H5"	20:T:65:LYS:HG3	2.01	0.42
1:A:342:C:N4	1:A:347:G:H1	2.16	0.42
1:A:586:C:C2'	1:A:587:G:H5'	2.49	0.42
1:A:924:C:O5'	1:A:924:C:H6	2.01	0.42
1:A:976:G:H22	1:A:1362:C:H2'	1.82	0.42
1:A:1052:U:C5'	23:Y:34:C:C6	3.02	0.42
1:A:1086:U:O5'	1:A:1086:U:C6	2.72	0.42
1:A:1107:C:H2'	1:A:1108:G:H5'	2.02	0.42
1:A:1257:U:H4'	1:A:1258:G:H8	1.84	0.42
1:A:1288:A:H1'	1:A:1352:C:HO2'	1.83	0.42
1:A:1345:U:C2	1:A:1377:A:C2	3.08	0.42
2:B:122:PHE:CZ	2:B:139:LYS:HG3	2.55	0.42
3:C:66:VAL:HG12	3:C:67:THR:H	1.83	0.42
3:C:87:LEU:HA	3:C:90:GLU:CB	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:LEU:HD11	3:C:99:VAL:HG23	2.00	0.42
3:C:148:GLY:O	3:C:202:ILE:HA	2.19	0.42
5:E:103:GLY:O	5:E:106:PRO:CD	2.64	0.42
6:F:10:LEU:HD11	6:F:59:TYR:CD2	2.53	0.42
6:F:62:TRP:CG	18:R:35:ARG:NH1	2.88	0.42
8:H:23:SER:HA	8:H:63:LEU:HD22	2.02	0.42
8:H:53:VAL:C	8:H:55:GLY:N	2.71	0.42
9:I:126:SER:O	9:I:128:ARG:N	2.52	0.42
11:K:34:ASP:CB	11:K:35:PRO:CD	2.98	0.42
12:L:56:ALA:HB2	12:L:70:ILE:HD11	2.00	0.42
13:M:45:VAL:HA	13:M:48:LEU:HG	2.01	0.42
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	2.01	0.42
1:A:442:C:C6	1:A:443:C:C5	3.07	0.42
1:A:492:G:C4	1:A:494:G:C8	3.07	0.42
1:A:736:C:H2'	1:A:737:A:C8	2.54	0.42
1:A:920:U:H2'	1:A:921:U:C6	2.55	0.42
1:A:1030:C:C2'	1:A:1030(A):G:C8	2.89	0.42
1:A:1098:C:H2'	1:A:1099:G:O4'	2.19	0.42
1:A:1320:C:O2	19:S:72:GLY:O	2.38	0.42
1:A:1415:G:C2	1:A:1416:G:C8	3.07	0.42
3:C:78:GLY:O	3:C:79:ARG:CB	2.67	0.42
6:F:64:GLN:O	6:F:64:GLN:HG2	2.19	0.42
8:H:20:TYR:CE2	8:H:75:ARG:HB3	2.54	0.42
9:I:84:ALA:C	9:I:86:VAL:N	2.73	0.42
10:J:78:ASN:O	10:J:82:ILE:HG13	2.20	0.42
14:N:9:LYS:HD3	14:N:9:LYS:O	2.20	0.42
14:N:37:PHE:C	14:N:39:LEU:N	2.72	0.42
15:O:8:LYS:O	15:O:12:ILE:HG13	2.19	0.42
16:P:28:ARG:HH11	16:P:28:ARG:CG	2.32	0.42
17:Q:36:ILE:O	17:Q:36:ILE:HG12	2.19	0.42
17:Q:90:ILE:O	17:Q:93:GLN:CB	2.67	0.42
17:Q:101:ARG:HD3	17:Q:102:GLY:H	1.84	0.42
19:S:5:LEU:HB3	19:S:6:LYS:H	1.64	0.42
1:A:119:A:H4'	1:A:120:A:O5'	2.20	0.42
1:A:247:G:OP2	17:Q:100:LYS:HG3	2.19	0.42
1:A:986:A:H4'	19:S:55:LYS:HG3	2.01	0.42
1:A:1074:G:O2'	2:B:103:THR:CG2	2.67	0.42
1:A:1447:G:H2'	1:A:1452:C:C5'	2.50	0.42
2:B:162:ILE:HG23	2:B:164:VAL:HG23	2.01	0.42
3:C:179:ARG:O	3:C:179:ARG:CD	2.68	0.42
4:D:64:LEU:HD13	4:D:64:LEU:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:TYR:HD1	4:D:68:TYR:H	1.67	0.42
4:D:150:GLU:CB	4:D:153:ARG:HH21	2.32	0.42
5:E:43:LEU:HD22	5:E:44:GLY:H	1.85	0.42
7:G:95:ARG:HG3	7:G:95:ARG:HH11	1.85	0.42
13:M:23:TYR:HB3	13:M:67:GLU:HA	2.02	0.42
20:T:97:ALA:O	20:T:99:LEU:N	2.53	0.42
1:A:420:U:H2'	1:A:422:C:C4	2.55	0.42
1:A:589:C:H2'	1:A:590:C:H6	1.85	0.42
1:A:656:C:H4'	15:O:62:GLN:NE2	2.34	0.42
1:A:1019:C:O2'	1:A:1020:U:H5'	2.20	0.42
1:A:1046:A:H2'	1:A:1047:G:H5'	2.02	0.42
1:A:1304:G:H1'	1:A:1333:A:H61	1.85	0.42
2:B:56:ARG:O	2:B:57:PHE:C	2.58	0.42
3:C:7:PRO:O	3:C:11:ARG:NE	2.48	0.42
4:D:24:GLU:HG2	4:D:25:ARG:N	2.34	0.42
4:D:157:LEU:HD23	4:D:157:LEU:O	2.20	0.42
5:E:64:ARG:O	5:E:65:ASN:HB3	2.20	0.42
7:G:39:ALA:O	7:G:40:ALA:C	2.57	0.42
12:L:46:LYS:CB	12:L:92:ASP:O	2.68	0.42
12:L:86:ARG:HH11	12:L:86:ARG:HG3	1.83	0.42
17:Q:9:VAL:HG22	17:Q:56:VAL:HG22	2.01	0.42
18:R:25:THR:HG22	18:R:25:THR:O	2.20	0.42
1:A:55:A:C2	1:A:56:U:C2	3.08	0.42
1:A:160:A:O2'	1:A:161:A:H5'	2.20	0.42
1:A:417:C:O5'	1:A:417:C:H6	2.02	0.42
1:A:539:A:OP1	12:L:114:LYS:HG2	2.20	0.42
1:A:623:C:O2'	1:A:624:C:H5'	2.19	0.42
1:A:685:G:C2	1:A:686:U:C4	3.07	0.42
1:A:1355:G:H2'	1:A:1356:G:H8	1.85	0.42
1:A:1400:C:O5'	1:A:1400:C:H6	2.03	0.42
2:B:25:ASN:HD22	2:B:26:PRO:N	2.17	0.42
2:B:38:GLY:C	2:B:39:ILE:HG13	2.40	0.42
2:B:111:ARG:O	2:B:149:LEU:CD1	2.67	0.42
3:C:121:ALA:HB2	3:C:187:ALA:HB1	2.00	0.42
3:C:188:LEU:C	3:C:188:LEU:HD13	2.40	0.42
4:D:57:ARG:HG2	4:D:202:LEU:HD22	2.02	0.42
4:D:59:ARG:NH2	4:D:62:GLN:HG3	2.34	0.42
4:D:116:GLN:NE2	4:D:157:LEU:HD11	2.35	0.42
5:E:99:GLY:O	5:E:117:ASP:HA	2.20	0.42
7:G:71:PRO:HD3	7:G:103:TRP:HZ3	1.85	0.42
7:G:89:MET:O	7:G:91:VAL:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:114:ARG:HG2	7:G:114:ARG:HH11	1.85	0.42
12:L:90:VAL:HG22	12:L:99:HIS:CE1	2.55	0.42
1:A:55:A:C2	1:A:56:U:N1	2.88	0.42
1:A:58:C:O2'	1:A:59:A:H5'	2.19	0.42
1:A:110:C:C4	1:A:111:G:C5	3.08	0.42
1:A:500:G:C6	1:A:546:G:C2	3.08	0.42
1:A:684:A:N6	1:A:685:G:C6	2.88	0.42
1:A:1049:U:O2	14:N:3:ARG:NH2	2.53	0.42
1:A:1202:G:H2'	1:A:1203:C:H5'	2.02	0.42
1:A:1312:G:O6	19:S:3:ARG:O	2.38	0.42
2:B:18:GLY:H	2:B:42:ILE:N	2.17	0.42
2:B:210:SER:C	2:B:212:GLN:N	2.72	0.42
3:C:90:GLU:O	3:C:93:LYS:HB2	2.20	0.42
3:C:108:ASN:C	3:C:110:ASN:N	2.70	0.42
3:C:207:VAL:O	3:C:207:VAL:HG12	2.20	0.42
4:D:17:VAL:HG12	4:D:18:LYS:N	2.34	0.42
4:D:126:ILE:CG2	4:D:127:THR:H	2.32	0.42
9:I:5:TYR:HH	9:I:16:ARG:HG2	1.85	0.42
9:I:110:GLU:HG2	9:I:113:LYS:HZ1	1.85	0.42
10:J:57:LYS:HD2	10:J:57:LYS:O	2.19	0.42
11:K:69:ALA:O	11:K:73:MET:HG2	2.20	0.42
11:K:90:GLY:O	11:K:93:GLN:N	2.51	0.42
15:O:63:ARG:HG2	15:O:67:LEU:HD12	2.01	0.42
19:S:15:LEU:HA	19:S:18:LYS:CB	2.33	0.42
1:A:10:A:OP2	5:E:126:ARG:HD3	2.20	0.42
1:A:81:U:HO2'	1:A:82:U:P	2.43	0.42
1:A:202:U:H4'	1:A:203:U:OP1	2.19	0.42
1:A:250:A:H2	1:A:274:A:C6	2.37	0.42
1:A:1014:A:H4'	19:S:14:HIS:ND1	2.35	0.42
1:A:1104:G:H2'	1:A:1105:A:C8	2.54	0.42
1:A:1199:U:H4'	10:J:54:PHE:CD1	2.54	0.42
1:A:1204:A:H2'	1:A:1205:U:O4'	2.20	0.42
1:A:1228:C:H2'	1:A:1229:A:H8	1.85	0.42
2:B:206:ASP:O	2:B:207:ALA:HB3	2.19	0.42
2:B:210:SER:O	2:B:211:ILE:C	2.58	0.42
3:C:67:THR:O	3:C:68:VAL:C	2.58	0.42
4:D:94:LEU:HD23	4:D:97:LEU:HD12	2.00	0.42
4:D:129:ASN:HB3	4:D:145:GLU:H	1.85	0.42
5:E:6:PHE:CZ	5:E:66:MET:HE1	2.55	0.42
7:G:47:CYS:O	7:G:50:ILE:N	2.52	0.42
9:I:102:LEU:N	9:I:102:LEU:CD2	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:102:ARG:O	13:M:102:ARG:HG3	2.19	0.42
18:R:76:LEU:HA	18:R:76:LEU:HD23	1.83	0.42
1:A:34:C:H1'	12:L:32:PHE:CZ	2.55	0.41
1:A:364:A:H61	12:L:28:LYS:NZ	2.17	0.41
1:A:370:C:O2	1:A:370:C:H2'	2.18	0.41
1:A:913:A:OP2	12:L:91:LYS:HE3	2.19	0.41
1:A:923:A:H8	1:A:923:A:O5'	2.03	0.41
1:A:977:A:OP2	1:A:977:A:H4'	2.20	0.41
1:A:1187:G:C2	1:A:1188:A:C4	3.07	0.41
1:A:1363:C:H3'	1:A:1363:C:OP2	2.19	0.41
1:A:1385:G:H2'	1:A:1386:G:O4'	2.19	0.41
1:A:1539:C:O2	1:A:1539:C:C2'	2.64	0.41
3:C:88:ARG:HA	3:C:101:LEU:CD1	2.46	0.41
5:E:79:GLU:O	8:H:104:ARG:CZ	2.68	0.41
7:G:14:PRO:HA	7:G:21:VAL:CG1	2.36	0.41
7:G:62:PHE:O	7:G:66:VAL:HG23	2.20	0.41
9:I:5:TYR:O	9:I:84:ALA:HA	2.18	0.41
9:I:33:PHE:O	9:I:35:GLU:N	2.53	0.41
9:I:63:ILE:HD13	9:I:77:ILE:HG23	2.01	0.41
9:I:100:GLY:C	9:I:102:LEU:HD23	2.40	0.41
10:J:24:VAL:HG21	10:J:72:VAL:CG1	2.49	0.41
13:M:37:THR:CG2	13:M:39:ILE:HG13	2.50	0.41
16:P:20:VAL:CG1	16:P:32:TYR:HB2	2.50	0.41
1:A:943:U:O2'	1:A:944:G:H5'	2.21	0.41
1:A:946:A:C2	1:A:1236:A:C2	3.08	0.41
1:A:1063:C:H2'	1:A:1064:G:C8	2.55	0.41
1:A:1254:C:OP1	10:J:45:ARG:HD2	2.20	0.41
1:A:1371:G:H2'	1:A:1372:U:C6	2.55	0.41
2:B:90:MET:CE	2:B:222:ILE:HD13	2.48	0.41
2:B:97:TRP:CZ3	2:B:99:GLY:HA2	2.49	0.41
2:B:169:LYS:HD3	2:B:169:LYS:C	2.40	0.41
2:B:187:LEU:HD12	2:B:205:ASP:HA	2.03	0.41
3:C:47:LEU:N	3:C:47:LEU:HD12	2.35	0.41
4:D:91:SER:O	4:D:92:VAL:C	2.58	0.41
4:D:191:ARG:O	4:D:191:ARG:NH1	2.50	0.41
8:H:30:ARG:HB3	8:H:30:ARG:HH11	1.85	0.41
10:J:74:ILE:HG22	10:J:75:ILE:N	2.36	0.41
11:K:16:SER:CB	11:K:79:SER:HB3	2.50	0.41
12:L:35:GLY:HA3	12:L:58:VAL:HG12	2.03	0.41
14:N:39:LEU:HB3	14:N:40:CYS:H	1.58	0.41
15:O:27:VAL:HG12	15:O:31:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:39:LEU:O	15:O:43:LEU:HG	2.20	0.41
19:S:11:VAL:HG21	19:S:41:VAL:HG13	2.02	0.41
19:S:66:MET:HA	19:S:69:HIS:CD2	2.56	0.41
1:A:67:C:H2'	1:A:68:G:C8	2.55	0.41
1:A:76:C:H2'	1:A:77:G:O5'	2.19	0.41
1:A:346:G:H2'	1:A:347:G:H5'	2.01	0.41
1:A:394:G:O2'	1:A:395:C:H5'	2.19	0.41
1:A:435:C:O2'	1:A:436:C:H5'	2.20	0.41
1:A:502:G:H2'	1:A:503:C:H6	1.85	0.41
1:A:1287:A:H2'	1:A:1288:A:H8	1.81	0.41
1:A:1298:C:H4'	1:A:1299:A:O4'	2.21	0.41
1:A:1316:G:N1	1:A:1319:A:OP2	2.46	0.41
1:A:1320:C:H1'	19:S:72:GLY:C	2.40	0.41
1:A:1447:G:N2	1:A:1459:C:O2	2.53	0.41
2:B:98:LEU:N	2:B:98:LEU:CD2	2.83	0.41
2:B:112:VAL:O	2:B:112:VAL:HG12	2.20	0.41
2:B:135:GLN:O	2:B:135:GLN:HG2	2.20	0.41
3:C:111:LEU:N	3:C:111:LEU:CD2	2.82	0.41
3:C:195:VAL:O	3:C:196:LEU:HD23	2.19	0.41
7:G:54:THR:CG2	7:G:55:GLY:N	2.83	0.41
8:H:4:ASP:OD2	8:H:7:ALA:CB	2.69	0.41
10:J:46:ARG:HG2	10:J:46:ARG:NH1	2.34	0.41
10:J:87:THR:O	10:J:88:LEU:HG	2.20	0.41
11:K:126:ARG:HH21	11:K:129:SER:HB3	1.82	0.41
13:M:70:LEU:O	13:M:74:VAL:HG23	2.21	0.41
13:M:105:THR:HB	13:M:106:ASN:H	1.69	0.41
14:N:40:CYS:SG	14:N:43:CYS:SG	3.09	0.41
15:O:3:ILE:HG13	15:O:38:ARG:CZ	2.50	0.41
15:O:21:ASP:OD2	15:O:24:SER:HB2	2.20	0.41
17:Q:11:VAL:C	17:Q:53:LEU:HD11	2.41	0.41
20:T:16:HIS:O	20:T:17:ARG:C	2.59	0.41
20:T:33:ILE:HD13	20:T:63:ILE:HA	2.01	0.41
1:A:171:A:O2'	1:A:172:A:H5'	2.20	0.41
1:A:251:G:C6	1:A:266:G:N1	2.89	0.41
1:A:426:G:P	4:D:36:ARG:HH21	2.43	0.41
1:A:429:U:O2	1:A:430:A:C8	2.74	0.41
1:A:922:G:C6	1:A:923:A:C6	3.09	0.41
1:A:1321:C:C5'	13:M:87:TYR:CE2	3.03	0.41
1:A:1328:C:H5"	13:M:28:ALA:HB1	2.01	0.41
2:B:188:ALA:HB1	2:B:192:SER:HG	1.83	0.41
2:B:191:ASP:C	2:B:191:ASP:OD2	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:LEU:HG	14:N:25:VAL:CG2	2.50	0.41
4:D:3:ARG:O	4:D:4:TYR:CB	2.68	0.41
5:E:101:ILE:HD12	5:E:119:LEU:HD21	2.02	0.41
7:G:135:VAL:O	7:G:138:LYS:HB3	2.20	0.41
7:G:136:LYS:C	7:G:138:LYS:N	2.74	0.41
9:I:55:ALA:O	9:I:56:LEU:HB3	2.21	0.41
10:J:40:LEU:HG	10:J:41:PRO:HD2	2.02	0.41
13:M:65:LYS:HD3	13:M:73:GLU:OE2	2.20	0.41
17:Q:95:TYR:CA	17:Q:98:LEU:HD11	2.44	0.41
17:Q:101:ARG:NE	17:Q:101:ARG:CA	2.83	0.41
19:S:28:LYS:CG	19:S:29:ARG:N	2.83	0.41
19:S:64:GLU:O	19:S:65:ASN:C	2.58	0.41
21:V:5:ASP:O	21:V:11:GLY:HA3	2.19	0.41
1:A:263:A:H2'	1:A:264:U:C6	2.55	0.41
1:A:320:C:H2'	1:A:321:A:C8	2.55	0.41
1:A:767:A:H2'	1:A:768:A:O4'	2.21	0.41
1:A:1131:G:H2'	1:A:1132:C:H6	1.86	0.41
1:A:1193:G:N2	1:A:1194:U:C2	2.89	0.41
1:A:1220:G:O3'	19:S:36:ARG:HD3	2.21	0.41
1:A:1272:G:C2'	1:A:1273:G:H5'	2.51	0.41
1:A:1288:A:C6	1:A:1289:A:C6	3.08	0.41
1:A:1396:A:H4'	1:A:1397:C:H5"	2.03	0.41
2:B:118:LEU:C	2:B:120:ALA:H	2.24	0.41
3:C:39:ILE:C	3:C:41:GLY:N	2.73	0.41
4:D:47:ARG:HG2	4:D:48:ALA:H	1.85	0.41
4:D:76:ARG:HD3	4:D:207:TYR:HE2	1.86	0.41
5:E:52:PRO:O	5:E:54:ALA:N	2.53	0.41
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.52	0.41
8:H:69:ARG:NH1	8:H:69:ARG:CB	2.60	0.41
9:I:90:PRO:C	9:I:92:TYR:H	2.22	0.41
11:K:21:ILE:HG22	11:K:22:HIS:N	2.35	0.41
11:K:90:GLY:O	11:K:93:GLN:HB3	2.21	0.41
13:M:23:TYR:O	13:M:25:ILE:N	2.54	0.41
15:O:10:LYS:C	15:O:10:LYS:CD	2.81	0.41
18:R:69:THR:O	18:R:72:ARG:HB3	2.19	0.41
1:A:22:G:H2'	1:A:23:C:H6	1.81	0.41
1:A:376:G:OP1	16:P:67:THR:HG21	2.21	0.41
1:A:529:G:H4'	1:A:533:A:N3	2.36	0.41
1:A:933:G:N7	7:G:3:ARG:NE	2.65	0.41
1:A:1044:A:H2'	1:A:1045:C:C4'	2.51	0.41
1:A:1250:A:H4'	9:I:68:GLY:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:SER:O	2:B:112:VAL:HB	2.21	0.41
2:B:164:VAL:O	2:B:186:ALA:HA	2.20	0.41
3:C:58:GLU:CB	10:J:92:THR:HG21	2.50	0.41
3:C:75:VAL:O	3:C:83:ARG:NH1	2.53	0.41
3:C:76:VAL:O	3:C:83:ARG:HB3	2.21	0.41
5:E:33:VAL:HG21	5:E:109:ILE:HG12	2.02	0.41
8:H:51:VAL:CG1	8:H:52:ASP:N	2.83	0.41
10:J:35:SER:HB2	10:J:73:ASP:HB3	2.03	0.41
11:K:40:ILE:CG2	11:K:41:THR:HG23	2.40	0.41
11:K:54:ARG:HA	11:K:57:THR:CG2	2.48	0.41
12:L:53:ARG:NH1	12:L:53:ARG:CG	2.84	0.41
12:L:60:LEU:C	12:L:62:SER:N	2.73	0.41
14:N:22:THR:O	14:N:33:VAL:HG21	2.21	0.41
15:O:55:GLY:O	15:O:58:MET:HB2	2.21	0.41
15:O:82:ILE:C	15:O:84:LYS:N	2.74	0.41
17:Q:48:GLU:HG2	17:Q:50:LYS:HG3	2.01	0.41
20:T:63:ILE:O	20:T:66:ALA:HB3	2.20	0.41
1:A:47:C:C6	1:A:365:U:H2'	2.55	0.41
1:A:127:G:HO2'	17:Q:2:PRO:N	2.19	0.41
1:A:175:C:C2	1:A:176:C:C6	3.09	0.41
1:A:188:C:O2	1:A:189:G:O2'	2.24	0.41
1:A:451:A:N7	1:A:481:G:C6	2.89	0.41
1:A:513:C:N4	1:A:538:G:H1	2.19	0.41
1:A:1036:G:H2'	1:A:1037:C:O4'	2.20	0.41
2:B:52:GLU:OE2	2:B:53:ARG:N	2.54	0.41
3:C:29:TYR:O	3:C:31:HIS:N	2.54	0.41
3:C:83:ARG:C	3:C:85:ARG:N	2.70	0.41
3:C:107:GLN:CD	3:C:107:GLN:N	2.74	0.41
7:G:23:VAL:O	7:G:24:THR:C	2.59	0.41
8:H:123:GLU:O	8:H:127:LEU:HD23	2.20	0.41
10:J:45:ARG:NH2	14:N:36:PHE:CB	2.84	0.41
10:J:57:LYS:HD2	10:J:57:LYS:C	2.41	0.41
18:R:58:LEU:HB3	18:R:62:GLU:HB2	2.02	0.41
1:A:112:G:O2'	1:A:113:G:H5'	2.21	0.41
1:A:643:C:H2'	1:A:644:G:H8	1.86	0.41
1:A:911:U:H2'	1:A:912:C:H6	1.80	0.41
1:A:965:A:C2	1:A:969:A:C2	3.08	0.41
1:A:1064:G:N2	1:A:1190:G:H2'	2.35	0.41
1:A:1277:C:O2'	1:A:1279:A:H1'	2.21	0.41
1:A:1524:C:H2'	1:A:1525:G:C8	2.55	0.41
2:B:141:GLU:O	2:B:142:LEU:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:VAL:HG12	3:C:83:ARG:NH2	2.36	0.41
6:F:25:ILE:O	6:F:28:ARG:HB3	2.21	0.41
8:H:4:ASP:CG	8:H:85:ARG:HH12	2.23	0.41
8:H:136:GLU:C	8:H:137:VAL:CG2	2.89	0.41
11:K:29:ILE:HD12	11:K:29:ILE:O	2.21	0.41
12:L:33:ARG:HA	12:L:33:ARG:HE	1.86	0.41
12:L:97:ARG:HB2	12:L:98:TYR:CE1	2.55	0.41
12:L:108:ALA:O	12:L:109:GLY:O	2.39	0.41
12:L:124:LYS:HD2	12:L:125:PRO:HD2	2.02	0.41
15:O:10:LYS:HG3	15:O:11:VAL:N	2.35	0.41
16:P:10:GLY:HA3	16:P:14:ASN:O	2.20	0.41
19:S:40:ILE:HD13	19:S:62:ILE:CD1	2.51	0.41
1:A:61:G:H22	1:A:379:C:H4'	1.85	0.41
1:A:192:U:H1'	20:T:103:GLY:HA2	2.02	0.41
1:A:380:G:C2	1:A:384:G:C6	3.08	0.41
1:A:481:G:H21	1:A:482:A:N6	2.19	0.41
1:A:536:C:O2	1:A:536:C:H2'	2.21	0.41
1:A:635:G:O2'	1:A:636:U:H5'	2.21	0.41
1:A:840:C:H4'	1:A:848:C:O2	2.19	0.41
1:A:851:G:O2'	1:A:852:G:H5'	2.21	0.41
1:A:969:A:C2'	1:A:970:C:H5'	2.50	0.41
1:A:1024:G:O2'	1:A:1025:U:H5'	2.20	0.41
1:A:1102:A:C6	1:A:1103:C:N4	2.89	0.41
1:A:1126:U:H6	1:A:1126:U:H3'	1.86	0.41
1:A:1227:A:H2'	1:A:1228:C:O5'	2.19	0.41
1:A:1255:G:H2'	1:A:1279:A:N6	2.33	0.41
1:A:1345:U:N3	1:A:1377:A:C2	2.88	0.41
1:A:1520:G:C2	1:A:1521:G:C5	3.09	0.41
2:B:87:ARG:NH2	2:B:219:VAL:HB	2.36	0.41
2:B:107:THR:O	2:B:109:SER:N	2.54	0.41
2:B:108:ILE:O	2:B:108:ILE:CG2	2.66	0.41
3:C:24:ALA:HB1	3:C:28:GLN:CB	2.50	0.41
3:C:44:GLU:CG	3:C:52:LEU:HD22	2.51	0.41
3:C:110:ASN:HD21	3:C:140:ARG:HD3	1.82	0.41
3:C:149:ALA:O	3:C:150:LYS:HB2	2.21	0.41
4:D:24:GLU:O	4:D:25:ARG:HB3	2.21	0.41
4:D:105:VAL:HG21	4:D:126:ILE:HG13	2.03	0.41
7:G:69:VAL:O	7:G:138:LYS:HG3	2.20	0.41
7:G:90:GLU:N	7:G:155:ARG:NH2	2.58	0.41
9:I:5:TYR:CG	9:I:6:GLY:N	2.88	0.41
12:L:89:ARG:NH2	12:L:97:ARG:NE	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:5:ALA:CB	13:M:22:ILE:HG23	2.51	0.41
13:M:40:ASN:HD22	13:M:41:PRO:HD2	1.86	0.41
13:M:114:ARG:NH1	13:M:114:ARG:HG2	2.36	0.41
16:P:2:VAL:O	16:P:2:VAL:HG22	2.20	0.41
17:Q:81:ARG:O	17:Q:81:ARG:CG	2.60	0.41
18:R:22:VAL:HB	18:R:56:THR:HA	2.02	0.41
20:T:84:LEU:C	20:T:86:ARG:N	2.74	0.41
1:A:939:G:C5'	7:G:102:ARG:HH22	2.20	0.41
1:A:980:C:H2'	1:A:981:U:H5'	2.03	0.41
1:A:1206:G:C6	1:A:1207:G:C5	3.09	0.41
1:A:1261:A:H62	1:A:1274:G:H21	1.69	0.41
1:A:1489:G:O2'	1:A:1490:C:H5"	2.21	0.41
2:B:51:LEU:HD22	2:B:55:PHE:CZ	2.56	0.41
2:B:213:LEU:HD23	2:B:214:ILE:CA	2.50	0.41
4:D:187:ARG:CZ	4:D:188:LEU:HD12	2.51	0.41
4:D:194:LEU:HD22	4:D:194:LEU:N	2.36	0.41
10:J:33:GLN:HB3	10:J:75:ILE:HD12	2.03	0.41
12:L:32:PHE:HB3	12:L:84:LEU:HD11	2.03	0.41
13:M:115:LYS:HE2	13:M:115:LYS:HB2	1.83	0.41
16:P:74:LEU:HG	16:P:79:VAL:HG21	2.03	0.41
1:A:163:C:O2'	1:A:164:U:H5'	2.21	0.40
1:A:255:G:H1'	17:Q:16:GLN:NE2	2.36	0.40
1:A:407:G:H5"	4:D:115:ARG:HB3	2.03	0.40
1:A:438:G:H4'	1:A:439:A:OP1	2.21	0.40
1:A:474:G:H21	1:A:475:G:C1'	2.33	0.40
1:A:474:G:OP2	1:A:475:G:O6	2.38	0.40
1:A:622:A:C8	1:A:623:C:C5	3.09	0.40
1:A:953:G:C6	1:A:954:G:C5	3.09	0.40
1:A:1073:U:H2'	1:A:1074:G:C8	2.55	0.40
1:A:1075:C:H5'	2:B:103:THR:HG21	2.04	0.40
1:A:1421:G:H1	1:A:1479:C:H42	1.69	0.40
2:B:41:ILE:O	2:B:41:ILE:HG22	2.21	0.40
2:B:73:THR:O	2:B:73:THR:HG22	2.20	0.40
2:B:156:LYS:O	2:B:156:LYS:CD	2.66	0.40
3:C:24:ALA:HB1	3:C:28:GLN:HB2	2.04	0.40
3:C:51:GLY:C	3:C:70:VAL:HG12	2.42	0.40
3:C:87:LEU:HD23	3:C:90:GLU:HB3	2.02	0.40
7:G:24:THR:HA	7:G:27:ILE:CD1	2.46	0.40
10:J:7:LYS:HE2	10:J:99:LYS:HZ1	1.85	0.40
14:N:3:ARG:O	14:N:4:LYS:C	2.57	0.40
17:Q:24:GLU:OE2	17:Q:37:LYS:HD2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:28:PRO:HA	17:Q:35:VAL:HA	2.03	0.40
17:Q:53:LEU:HD12	17:Q:53:LEU:HA	1.86	0.40
1:A:284:G:O2'	1:A:285:G:H5'	2.22	0.40
1:A:385:C:H2'	1:A:386:C:H6	1.84	0.40
1:A:529:G:O4'	1:A:533:A:C2	2.74	0.40
1:A:962:C:H2'	1:A:963:G:O4'	2.21	0.40
1:A:1038:C:H2'	1:A:1039:C:H6	1.87	0.40
1:A:1052:U:H5'	23:Y:34:C:C5	2.55	0.40
1:A:1443:G:C4'	1:A:1446:A:C5'	2.98	0.40
2:B:124:SER:HB2	2:B:125:PRO:HD2	2.02	0.40
8:H:119:LEU:HD12	8:H:124:ALA:CA	2.51	0.40
10:J:7:LYS:HZ1	10:J:99:LYS:HZ2	1.69	0.40
10:J:8:LEU:HD13	10:J:20:ALA:CB	2.51	0.40
14:N:29:ARG:NH1	14:N:29:ARG:HB3	2.37	0.40
16:P:43:LYS:HA	16:P:48:TRP:HB3	2.03	0.40
21:V:13:ILE:HG22	21:V:14:TRP:N	2.35	0.40
1:A:35:G:N2	12:L:118:SER:CB	2.79	0.40
1:A:79:G:H2'	1:A:79:G:N3	2.36	0.40
1:A:118:U:H3'	1:A:288:A:H61	1.87	0.40
1:A:162:A:C5	1:A:163:C:H1'	2.57	0.40
1:A:385:C:H2'	1:A:386:C:C6	2.56	0.40
1:A:689:C:H2'	1:A:690:G:O4'	2.20	0.40
1:A:1004:A:H2'	1:A:1005:A:C4'	2.51	0.40
1:A:1103:C:H2'	1:A:1104:G:O4'	2.21	0.40
1:A:1203:C:H6	1:A:1203:C:O5'	2.05	0.40
1:A:1320:C:OP1	19:S:70:LYS:CE	2.70	0.40
1:A:1321:C:C6	1:A:1322:C:C6	3.09	0.40
1:A:1497:G:H2'	1:A:1498:U:C5'	2.50	0.40
2:B:137:ARG:HH11	2:B:138:LEU:CG	2.35	0.40
4:D:52:SER:O	4:D:55:ALA:N	2.53	0.40
4:D:190:ASP:O	4:D:191:ARG:C	2.59	0.40
16:P:67:THR:CG2	16:P:68:ASP:N	2.84	0.40
17:Q:66:SER:OG	17:Q:67:LYS:N	2.54	0.40
17:Q:72:ARG:HE	17:Q:72:ARG:HB2	1.71	0.40
19:S:77:THR:CG2	19:S:78:ARG:H	2.31	0.40
20:T:73:HIS:C	20:T:74:LYS:HG2	2.41	0.40
1:A:165:C:O2'	1:A:166:G:H5'	2.22	0.40
1:A:378:G:C6	1:A:379:C:C4	3.09	0.40
1:A:428:G:OP2	4:D:7:PRO:HG3	2.21	0.40
1:A:442:C:H2'	1:A:443:C:C6	2.56	0.40
1:A:551:U:H2'	1:A:552:U:H6	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:A:H2'	1:A:701:C:N4	2.36	0.40
1:A:824:C:H2'	1:A:825:G:H8	1.86	0.40
1:A:1049:U:O2'	1:A:1050:G:OP2	2.29	0.40
1:A:1436:U:O2'	1:A:1437:C:H5'	2.22	0.40
1:A:1461:G:H2'	1:A:1462:G:H8	1.86	0.40
1:A:1526:G:H2'	1:A:1527:C:H6	1.87	0.40
2:B:46:LYS:CA	2:B:49:GLU:OE1	2.69	0.40
2:B:191:ASP:OD2	2:B:192:SER:N	2.54	0.40
2:B:231:GLU:CD	2:B:231:GLU:H	2.24	0.40
3:C:151:VAL:CG1	3:C:152:ILE:N	2.83	0.40
4:D:162:LEU:HD13	4:D:181:MET:CE	2.51	0.40
5:E:72:GLN:C	5:E:74:GLY:H	2.24	0.40
7:G:72:ARG:HH11	7:G:72:ARG:HG2	1.87	0.40
7:G:148:ASN:O	7:G:150:ALA:N	2.54	0.40
8:H:122:ARG:CZ	8:H:122:ARG:HB2	2.51	0.40
8:H:136:GLU:O	8:H:137:VAL:CG2	2.69	0.40
9:I:63:ILE:HG22	9:I:65:VAL:N	2.33	0.40
9:I:118:LYS:C	9:I:120:ARG:H	2.25	0.40
13:M:4:ILE:HD11	13:M:56:LEU:HD12	2.04	0.40
14:N:51:GLY:C	14:N:53:LEU:H	2.25	0.40
19:S:30:LEU:HD22	19:S:31:ILE:H	1.86	0.40
1:A:64:G:H4'	1:A:65:U:H3'	2.04	0.40
1:A:143:A:O5'	1:A:143:A:H8	2.05	0.40
1:A:235:C:C5'	17:Q:70:ARG:HD3	2.52	0.40
1:A:476:G:C2	1:A:477:G:N7	2.90	0.40
1:A:679:C:H2'	1:A:680:C:C6	2.56	0.40
1:A:1135:U:H4'	1:A:1136:U:H5	1.80	0.40
1:A:1303:C:H2'	1:A:1304:G:H5'	2.04	0.40
1:A:1366:C:C6	1:A:1367:C:C5	3.09	0.40
1:A:1447:G:H2'	1:A:1452:C:H5'	2.03	0.40
2:B:197:VAL:HB	2:B:200:ILE:CD1	2.39	0.40
3:C:21:ARG:HE	3:C:21:ARG:HB2	1.71	0.40
3:C:29:TYR:C	3:C:31:HIS:N	2.75	0.40
3:C:132:ARG:O	3:C:133:ALA:C	2.60	0.40
4:D:57:ARG:HE	4:D:205:GLU:HB3	1.87	0.40
10:J:5:ARG:N	10:J:100:THR:HA	2.26	0.40
11:K:34:ASP:CB	11:K:35:PRO:HD2	2.45	0.40
12:L:35:GLY:HA3	12:L:58:VAL:HG11	2.04	0.40
12:L:43:VAL:HG21	12:L:55:VAL:HG11	2.03	0.40
12:L:78:GLN:O	12:L:80:HIS:N	2.50	0.40
12:L:117:ARG:O	12:L:118:SER:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:14:ASN:N	16:P:15:PRO:CD	2.84	0.40
17:Q:66:SER:HB3	17:Q:69:LYS:CB	2.46	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%)	149 (64%)	60 (26%)	24 (10%)	0	3
3	C	205/239 (86%)	119 (58%)	53 (26%)	33 (16%)	0	0
4	D	206/209 (99%)	131 (64%)	54 (26%)	21 (10%)	0	3
5	E	149/162 (92%)	124 (83%)	15 (10%)	10 (7%)	1	9
6	F	99/101 (98%)	73 (74%)	19 (19%)	7 (7%)	1	8
7	G	153/156 (98%)	100 (65%)	35 (23%)	18 (12%)	0	2
8	H	136/138 (99%)	107 (79%)	19 (14%)	10 (7%)	1	7
9	I	125/128 (98%)	78 (62%)	34 (27%)	13 (10%)	0	3
10	J	97/105 (92%)	53 (55%)	29 (30%)	15 (16%)	0	1
11	K	117/129 (91%)	85 (73%)	18 (15%)	14 (12%)	0	2
12	L	123/135 (91%)	92 (75%)	16 (13%)	15 (12%)	0	2
13	M	123/126 (98%)	89 (72%)	21 (17%)	13 (11%)	0	2
14	N	58/61 (95%)	33 (57%)	19 (33%)	6 (10%)	0	3
15	O	86/89 (97%)	60 (70%)	23 (27%)	3 (4%)	3	24
16	P	82/88 (93%)	62 (76%)	16 (20%)	4 (5%)	2	17
17	Q	102/105 (97%)	82 (80%)	10 (10%)	10 (10%)	0	3
18	R	71/88 (81%)	49 (69%)	15 (21%)	7 (10%)	0	3
19	S	79/93 (85%)	50 (63%)	15 (19%)	14 (18%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	T	97/106 (92%)	67 (69%)	19 (20%)	11 (11%)	0 2
21	V	23/27 (85%)	18 (78%)	2 (9%)	3 (13%)	0 1
All	All	2364/2541 (93%)	1621 (69%)	492 (21%)	251 (11%)	0 2

All (251) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	17	PHE
2	B	23	ARG
2	B	95	GLN
2	B	98	LEU
3	C	15	THR
3	C	61	ALA
3	C	75	VAL
3	C	79	ARG
3	C	130	VAL
3	C	154	SER
3	C	155	GLY
3	C	156	ARG
3	C	168	ALA
3	C	179	ARG
4	D	30	LYS
4	D	88	VAL
4	D	110	PHE
4	D	129	ASN
5	E	6	PHE
5	E	153	LYS
6	F	37	VAL
6	F	64	GLN
6	F	70	ASP
7	G	4	ARG
7	G	5	ARG
7	G	7	ALA
7	G	59	LEU
7	G	60	LYS
8	H	83	ILE
8	H	105	ARG
9	I	55	ALA
9	I	65	VAL
10	J	34	VAL

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Mol	Chain	Res	Type
10	J	54	PHE
10	J	55	LYS
11	K	48	ILE
11	K	91	ARG
11	K	101	SER
12	L	27	LEU
12	L	37	CYS
12	L	41	ARG
12	L	47	LYS
12	L	80	HIS
13	M	23	TYR
13	M	106	ASN
14	N	15	LYS
14	N	19	ARG
14	N	30	ALA
15	O	84	LYS
17	Q	49	GLU
17	Q	81	ARG
17	Q	101	ARG
18	R	22	VAL
18	R	86	VAL
19	S	5	LEU
19	S	9	VAL
19	S	32	LYS
19	S	47	HIS
19	S	65	ASN
20	T	49	ALA
20	T	50	GLU
20	T	73	HIS
21	V	3	LYS
2	B	9	GLU
2	B	13	ALA
2	B	18	GLY
2	B	123	ALA
2	B	128	GLU
2	B	159	PRO
2	B	165	VAL
3	C	3	ASN
3	C	68	VAL
3	C	74	GLY
3	C	84	ILE
3	C	128	PHE

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Mol	Chain	Res	Type
3	C	146	ALA
4	D	4	TYR
4	D	20	TYR
4	D	26	CYS
4	D	29	PRO
4	D	56	VAL
4	D	105	VAL
4	D	150	GLU
5	E	104	ALA
5	E	107	ARG
6	F	65	VAL
6	F	66	GLU
6	F	72	VAL
7	G	6	ARG
7	G	78	ARG
7	G	80	VAL
7	G	90	GLU
7	G	150	ALA
8	H	91	ARG
8	H	137	VAL
9	I	33	PHE
9	I	34	ASN
9	I	58	ARG
9	I	127	LYS
10	J	36	GLY
10	J	51	ARG
10	J	65	LEU
10	J	82	ILE
11	K	39	PRO
11	K	40	ILE
11	K	52	GLY
11	K	100	ALA
11	K	102	GLY
12	L	51	ALA
12	L	56	ALA
12	L	79	GLU
12	L	109	GLY
13	M	7	VAL
13	M	24	GLY
13	M	30	ALA
16	P	10	GLY
17	Q	50	LYS

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Mol	Chain	Res	Type
17	Q	80	GLY
17	Q	98	LEU
17	Q	99	SER
19	S	27	GLU
20	T	9	ASN
20	T	11	SER
20	T	103	GLY
2	B	52	GLU
2	B	74	LYS
2	B	83	MET
2	B	142	LEU
2	B	152	PHE
2	B	195	ASP
3	C	16	ARG
3	C	35	GLU
3	C	77	ILE
3	C	81	GLY
3	C	96	GLY
3	C	160	ALA
4	D	151	LYS
4	D	153	ARG
5	E	78	HIS
7	G	33	ASP
7	G	104	LEU
7	G	108	ALA
7	G	137	LYS
8	H	135	CYS
9	I	108	VAL
10	J	30	SER
10	J	81	THR
10	J	90	LEU
11	K	35	PRO
11	K	47	VAL
11	K	117	ASN
13	M	68	GLY
13	M	88	ARG
13	M	118	ALA
13	M	120	LYS
14	N	14	PRO
15	O	83	GLU
17	Q	97	SER
18	R	21	LYS

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Mol	Chain	Res	Type
18	R	54	ARG
18	R	63	GLN
19	S	24	ALA
19	S	42	PRO
19	S	64	GLU
20	T	99	LEU
21	V	25	LYS
2	B	237	ALA
2	B	238	LEU
3	C	45	LYS
3	C	66	VAL
3	C	119	ARG
3	C	132	ARG
4	D	9	CYS
4	D	42	GLN
4	D	206	PHE
5	E	53	LEU
5	E	129	ILE
6	F	39	LYS
7	G	22	LEU
7	G	100	ALA
7	G	155	ARG
8	H	50	ARG
9	I	25	LYS
9	I	41	VAL
9	I	101	PHE
10	J	60	ARG
10	J	73	ASP
10	J	76	ASN
11	K	15	ALA
12	L	29	GLY
12	L	112	ASP
12	L	123	LYS
13	M	123	ALA
14	N	36	PHE
16	P	34	GLU
16	P	52	ASP
17	Q	47	PRO
19	S	30	LEU
19	S	55	LYS
20	T	95	ALA
20	T	97	ALA

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Mol	Chain	Res	Type
2	B	130	ARG
3	C	14	ILE
3	C	32	LEU
3	C	40	ARG
4	D	156	GLU
5	E	128	PRO
7	G	18	TYR
8	H	73	ASP
8	H	126	LYS
9	I	43	ALA
9	I	61	ALA
12	L	30	ALA
18	R	19	LYS
19	S	43	GLU
20	T	54	LYS
21	V	13	ILE
2	B	108	ILE
3	C	133	ALA
4	D	157	LEU
8	H	103	VAL
10	J	72	VAL
13	M	117	VAL
15	O	38	ARG
4	D	8	VAL
5	E	52	PRO
9	I	6	GLY
12	L	55	VAL
17	Q	23	VAL
19	S	26	GLY
20	T	98	PRO
2	B	15	VAL
5	E	22	GLY
8	H	51	VAL
13	M	6	GLY
13	M	60	VAL
14	N	28	GLY
18	R	48	GLY
3	C	153	VAL
12	L	40	VAL
16	P	36	ILE
19	S	68	GLY
2	B	208	ILE

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Mol	Chain	Res	Type
3	C	73	PRO
3	C	108	ASN
4	D	5	ILE
11	K	76	GLY
4	D	172	PRO
10	J	24	VAL
11	K	118	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	182 (90%)	20 (10%)	8	30
3	C	160/188 (85%)	151 (94%)	9 (6%)	21	57
4	D	180/181 (99%)	165 (92%)	15 (8%)	11	40
5	E	115/123 (94%)	98 (85%)	17 (15%)	3	14
6	F	90/90 (100%)	84 (93%)	6 (7%)	16	50
7	G	126/127 (99%)	115 (91%)	11 (9%)	10	37
8	H	119/119 (100%)	104 (87%)	15 (13%)	4	21
9	I	98/99 (99%)	94 (96%)	4 (4%)	30	66
10	J	87/92 (95%)	80 (92%)	7 (8%)	12	42
11	K	90/99 (91%)	85 (94%)	5 (6%)	21	57
12	L	104/111 (94%)	96 (92%)	8 (8%)	13	44
13	M	100/101 (99%)	90 (90%)	10 (10%)	7	30
14	N	49/50 (98%)	44 (90%)	5 (10%)	7	29
15	O	79/80 (99%)	74 (94%)	5 (6%)	18	52
16	P	72/74 (97%)	68 (94%)	4 (6%)	21	57
17	Q	96/97 (99%)	90 (94%)	6 (6%)	18	52
18	R	64/77 (83%)	60 (94%)	4 (6%)	18	52
19	S	71/80 (89%)	69 (97%)	2 (3%)	43	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	T	76/82 (93%)	68 (90%)	8 (10%)	7 28
21	V	19/22 (86%)	19 (100%)	0	100 100
All	All	1997/2112 (95%)	1836 (92%)	161 (8%)	11 42

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	23	ARG
2	B	24	TRP
2	B	25	ASN
2	B	71	VAL
2	B	92	TYR
2	B	98	LEU
2	B	111	ARG
2	B	144	ARG
2	B	154	LEU
2	B	155	LEU
2	B	156	LYS
2	B	162	ILE
2	B	178	ARG
2	B	189	ASP
2	B	196	LEU
2	B	198	ASP
2	B	212	GLN
2	B	224	GLN
2	B	231	GLU
3	C	3	ASN
3	C	29	TYR
3	C	34	LEU
3	C	56	ASP
3	C	58	GLU
3	C	111	LEU
3	C	128	PHE
3	C	167	TRP
3	C	193	TYR
4	D	29	PRO
4	D	34	GLU
4	D	38	TYR
4	D	50	ARG
4	D	53	ASP

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Mol	Chain	Res	Type
4	D	58	LEU
4	D	59	ARG
4	D	62	GLN
4	D	66	ARG
4	D	68	TYR
4	D	110	PHE
4	D	129	ASN
4	D	131	ARG
4	D	199	ASN
4	D	200	GLU
5	E	10	MET
5	E	12	LEU
5	E	14	ARG
5	E	24	ARG
5	E	41	VAL
5	E	43	LEU
5	E	52	PRO
5	E	61	TYR
5	E	64	ARG
5	E	73	ASN
5	E	75	THR
5	E	79	GLU
5	E	80	ILE
5	E	100	VAL
5	E	121	LYS
5	E	127	ASN
5	E	150	ARG
6	F	14	LEU
6	F	24	GLU
6	F	43	LEU
6	F	47	ARG
6	F	69	GLU
6	F	79	LEU
7	G	12	LEU
7	G	16	LEU
7	G	37	ASN
7	G	38	LEU
7	G	72	ARG
7	G	97	GLN
7	G	111	ARG
7	G	113	GLU
7	G	126	ASP

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Mol	Chain	Res	Type
7	G	140	ASP
7	G	156	TRP
8	H	5	PRO
8	H	14	ARG
8	H	25	ASP
8	H	26	VAL
8	H	39	LEU
8	H	50	ARG
8	H	54	ASP
8	H	56	LYS
8	H	65	TYR
8	H	67	PRO
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	112	LEU
8	H	119	LEU
9	I	2	GLU
9	I	23	ASN
9	I	104	ARG
9	I	125	TYR
10	J	21	GLN
10	J	46	ARG
10	J	56	HIS
10	J	57	LYS
10	J	58	ASP
10	J	65	LEU
10	J	85	LEU
11	K	12	ARG
11	K	33	THR
11	K	35	PRO
11	K	54	ARG
11	K	93	GLN
12	L	17	LYS
12	L	48	PRO
12	L	53	ARG
12	L	62	SER
12	L	93	LEU
12	L	98	TYR
12	L	99	HIS
12	L	126	LYS
13	M	11	ARG

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Mol	Chain	Res	Type
13	M	40	ASN
13	M	44	ARG
13	M	48	LEU
13	M	66	LEU
13	M	81	LEU
13	M	102	ARG
13	M	110	ARG
13	M	115	LYS
13	M	125	ARG
14	N	8	GLU
14	N	12	ARG
14	N	26	ARG
14	N	27	CYS
14	N	41	ARG
15	O	10	LYS
15	O	34	LEU
15	O	64	ARG
15	O	65	ARG
15	O	70	LEU
16	P	2	VAL
16	P	26	ARG
16	P	52	ASP
16	P	55	ARG
17	Q	25	ARG
17	Q	36	ILE
17	Q	38	ARG
17	Q	60	ILE
17	Q	98	LEU
17	Q	101	ARG
18	R	36	ASN
18	R	54	ARG
18	R	56	THR
18	R	87	ARG
19	S	12	ASP
19	S	79	THR
20	T	10	LEU
20	T	62	LEU
20	T	64	ASP
20	T	68	LYS
20	T	73	HIS
20	T	75	ASN
20	T	79	ARG

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Mol	Chain	Res	Type
20	T	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	HIS
2	B	25	ASN
2	B	40	HIS
2	B	78	GLN
2	B	146	GLN
2	B	212	GLN
3	C	3	ASN
3	C	6	HIS
3	C	31	HIS
3	C	69	HIS
3	C	110	ASN
3	C	118	GLN
3	C	139	GLN
3	C	176	HIS
4	D	62	GLN
4	D	129	ASN
4	D	199	ASN
5	E	72	GLN
5	E	73	ASN
6	F	18	GLN
6	F	27	GLN
6	F	64	GLN
6	F	94	GLN
6	F	100	ASN
7	G	37	ASN
7	G	68	ASN
7	G	86	GLN
7	G	97	GLN
7	G	106	GLN
8	H	78	GLN
9	I	23	ASN
10	J	56	HIS
10	J	84	GLN
11	K	22	HIS
11	K	117	ASN
12	L	49	ASN
12	L	78	GLN

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Mol	Chain	Res	Type
12	L	99	HIS
13	M	12	ASN
13	M	40	ASN
13	M	62	ASN
14	N	49	HIS
14	N	52	GLN
15	O	37	ASN
16	P	16	HIS
16	P	76	GLN
17	Q	16	GLN
17	Q	26	GLN
18	R	36	ASN
19	S	23	ASN
19	S	53	ASN
19	S	69	HIS
20	T	16	HIS
20	T	42	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1472/1523 (96%)	218 (14%)	66 (4%)
22	X	3/4 (75%)	1 (33%)	0
23	Y	7/18 (38%)	4 (57%)	0
All	All	1482/1545 (95%)	223 (15%)	66 (4%)

All (223) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	52	G
1	A	61	G
1	A	63	C
1	A	70	G

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Mol	Chain	Res	Type
1	A	73	C
1	A	76	C
1	A	82	U
1	A	90	U
1	A	92	C
1	A	93	G
1	A	97	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129	U
1	A	131	C
1	A	144	G
1	A	163	C
1	A	189	G
1	A	190	C
1	A	192	U
1	A	193	C
1	A	195	A
1	A	196	A
1	A	197	A
1	A	198	G
1	A	202	U
1	A	203	U
1	A	204	U
1	A	217	C
1	A	220	G
1	A	244	U
1	A	245	C
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	306	G
1	A	328	C
1	A	332	G
1	A	345	C
1	A	350	G

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Mol	Chain	Res	Type
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	397	A
1	A	412	A
1	A	413	G
1	A	421	U
1	A	428	G
1	A	429	U
1	A	438	G
1	A	439	A
1	A	443	C
1	A	452	A
1	A	458	C
1	A	461	C
1	A	474	G
1	A	477	G
1	A	480	U
1	A	485	G
1	A	511	C
1	A	518	C
1	A	532	A
1	A	533	A
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	653	A
1	A	665	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	723	U

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Mol	Chain	Res	Type
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	787	A
1	A	792	A
1	A	793	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	848	C
1	A	859	A
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	945	G
1	A	960	U
1	A	965	A
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	992	U
1	A	994	A
1	A	1005	A
1	A	1006	A
1	A	1006(A)	C
1	A	1007	C
1	A	1023	G
1	A	1024	G
1	A	1026	G
1	A	1031	G

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Mol	Chain	Res	Type
1	A	1033	G
1	A	1045	C
1	A	1050	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
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	1146	A
1	A	1152	A
1	A	1159	U
1	A	1168	A
1	A	1183	A
1	A	1184	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1215	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1238	A
1	A	1257	U
1	A	1258	G
1	A	1279	A
1	A	1280	A

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Mol	Chain	Res	Type
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	1302	U
1	A	1305	G
1	A	1331	G
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1360	A
1	A	1362	C
1	A	1363	C
1	A	1370	G
1	A	1398	A
1	A	1401	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1452	C
1	A	1459	C
1	A	1490	C
1	A	1492	A
1	A	1493	A
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1534	A
22	X	4	G
23	Y	34	C
23	Y	35	C
23	Y	39	A

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Mol	Chain	Res	Type
23	Y	40	U

All (66) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	48	C
1	A	51	A
1	A	60	A
1	A	70	G
1	A	73	C
1	A	81	U
1	A	115	G
1	A	119	A
1	A	197	A
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	344	A
1	A	353	A
1	A	366	C
1	A	372	C
1	A	428	G
1	A	438	G
1	A	442	C
1	A	484	G
1	A	533	A
1	A	560	U
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	913	A
1	A	965	A
1	A	975	A
1	A	993	G
1	A	1006	A

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Mol	Chain	Res	Type
1	A	1049	U
1	A	1054	C
1	A	1065	U
1	A	1067	A
1	A	1101	A
1	A	1145	C
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1201	A
1	A	1214	C
1	A	1224	G
1	A	1226	C
1	A	1256	A
1	A	1257	U
1	A	1279	A
1	A	1281	U
1	A	1285	A
1	A	1301	U
1	A	1346	A
1	A	1347	G
1	A	1397	C
1	A	1452	C
1	A	1490	C
1	A	1498	U
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1528	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 81 ligands modelled in this entry, 80 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	3001	-	44,45,45	1.40	7 (15%)	63,67,67	1.20	7 (11%)

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	3001	-	-	1/18/94/94	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	3001	PAR	C52-C42	3.56	1.59	1.52
24	A	3001	PAR	O54-C14	2.80	1.49	1.41
24	A	3001	PAR	C11-C21	2.77	1.57	1.52
24	A	3001	PAR	C31-C21	2.59	1.56	1.53
24	A	3001	PAR	O51-C11	2.20	1.47	1.41
24	A	3001	PAR	C34-C24	2.11	1.56	1.53
24	A	3001	PAR	C14-C24	2.01	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	3001	PAR	O33-C14-C24	3.52	113.84	108.08
24	A	3001	PAR	O54-C54-C64	3.41	112.62	106.07
24	A	3001	PAR	C14-O54-C54	3.10	119.78	113.72
24	A	3001	PAR	O11-C11-C21	2.99	112.97	108.08
24	A	3001	PAR	O52-C13-O43	-2.64	108.67	111.37
24	A	3001	PAR	C11-O51-C51	2.43	118.47	113.72
24	A	3001	PAR	C22-C32-C42	2.08	114.59	109.50

There are no chirality outliers.

All (1) torsion outliers are listed below:

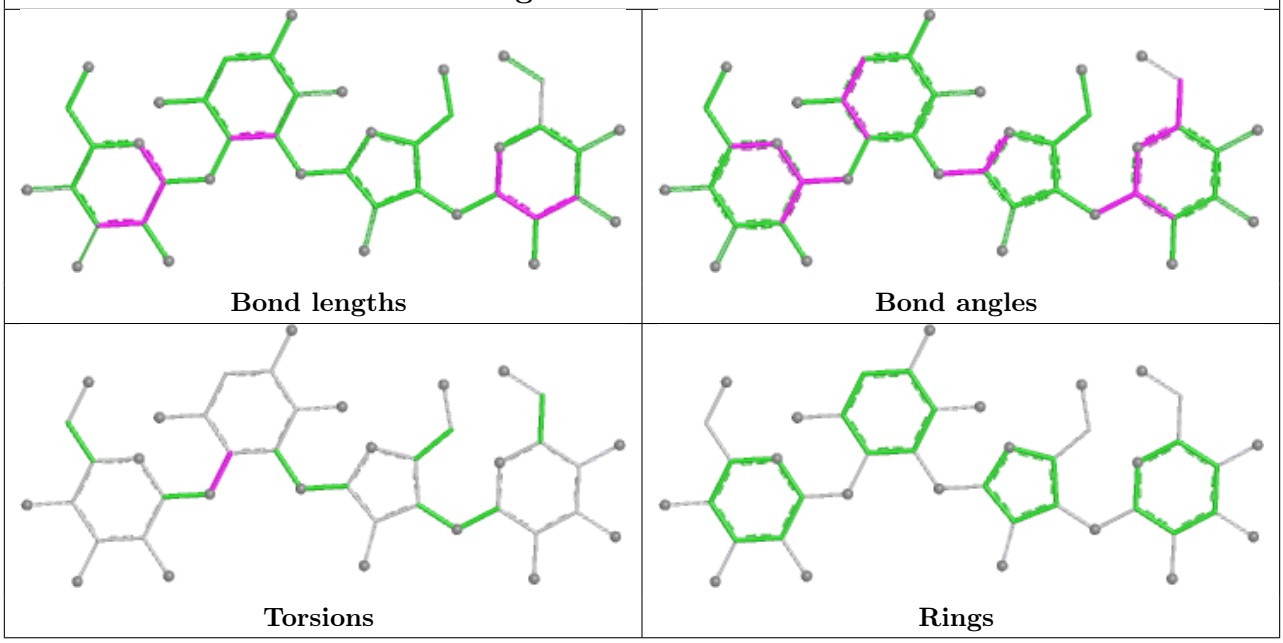
Mol	Chain	Res	Type	Atoms
24	A	3001	PAR	C52-C42-O11-C11

There are no ring outliers.

No monomer is involved in short contacts.

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 3001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1484/1523 (97%)	0.78	108 (7%)	15	9	40, 86, 171, 201	0
2	B	235/256 (91%)	0.20	14 (5%)	21	12	50, 117, 152, 155	0
3	C	207/239 (86%)	0.45	23 (11%)	5	3	61, 123, 153, 155	0
4	D	208/209 (99%)	0.13	10 (4%)	30	18	57, 101, 143, 155	0
5	E	151/162 (93%)	-0.19	0	100	100	43, 76, 119, 149	0
6	F	101/101 (100%)	0.33	3 (2%)	50	34	64, 116, 146, 151	0
7	G	155/156 (99%)	0.26	6 (3%)	39	25	63, 121, 153, 155	0
8	H	138/138 (100%)	-0.20	0	100	100	39, 67, 111, 132	0
9	I	127/128 (99%)	0.36	8 (6%)	20	11	54, 123, 155, 155	0
10	J	99/105 (94%)	0.95	14 (14%)	2	2	70, 139, 155, 155	0
11	K	119/129 (92%)	0.09	3 (2%)	57	43	44, 89, 134, 148	0
12	L	125/135 (92%)	0.15	2 (1%)	72	59	38, 96, 137, 155	0
13	M	125/126 (99%)	0.59	12 (9%)	8	4	68, 108, 144, 155	0
14	N	60/61 (98%)	0.29	3 (5%)	28	16	74, 116, 145, 155	0
15	O	88/89 (98%)	-0.03	1 (1%)	80	69	49, 88, 136, 145	0
16	P	84/88 (95%)	0.05	1 (1%)	79	67	46, 75, 109, 154	0
17	Q	104/105 (99%)	0.02	3 (2%)	51	36	47, 76, 132, 155	0
18	R	73/88 (82%)	0.10	4 (5%)	25	14	52, 95, 141, 155	0
19	S	81/93 (87%)	0.56	9 (11%)	5	3	95, 136, 154, 155	0
20	T	99/106 (93%)	0.29	6 (6%)	21	12	51, 84, 139, 155	0
21	V	25/27 (92%)	0.57	1 (4%)	38	25	63, 89, 132, 152	0
22	X	4/4 (100%)	0.48	0	100	100	102, 111, 115, 128	0
23	Y	8/18 (44%)	1.16	1 (12%)	3	2	104, 144, 155, 155	0
All	All	3900/4086 (95%)	0.44	232 (5%)	22	13	38, 96, 154, 201	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	125	ARG	8.6
1	A	1447	G	7.9
4	D	25	ARG	7.9
1	A	1166	G	6.9
1	A	1452	C	6.8
13	M	118	ALA	6.7
1	A	73	C	6.6
20	T	103	GLY	6.5
1	A	1024	G	6.5
13	M	124	PRO	6.4
19	S	82	GLY	5.8
10	J	10	GLY	5.6
1	A	1005	A	5.5
13	M	123	ALA	5.5
1	A	160	A	5.4
1	A	461	C	5.1
13	M	126	LYS	5.1
1	A	1003	G	5.1
1	A	1260	C	5.0
1	A	1534	A	5.0
1	A	1006	A	5.0
1	A	1135	U	5.0
1	A	428	G	4.9
19	S	27	GLU	4.8
1	A	530	G	4.8
1	A	1446	A	4.8
13	M	7	VAL	4.7
7	G	73	MET	4.7
4	D	42	GLN	4.6
10	J	29	ARG	4.6
13	M	122	LYS	4.5
2	B	19	HIS	4.5
1	A	1029	C	4.5
1	A	1129	C	4.4
10	J	27	ALA	4.4
10	J	88	LEU	4.3
1	A	1023	G	4.3
1	A	496	A	4.2
1	A	1001	A	4.2
10	J	34	VAL	4.1
4	D	23	GLY	4.1
21	V	26	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
9	I	92	TYR	4.1
10	J	80	LYS	4.0
3	C	99	VAL	4.0
11	K	35	PRO	4.0
1	A	1028	C	3.9
1	A	1036	G	3.9
1	A	1001(A)	G	3.9
1	A	1131	G	3.8
1	A	1138	G	3.8
1	A	1004	A	3.8
1	A	1030	C	3.8
1	A	1274	G	3.8
1	A	1276	G	3.7
3	C	70	VAL	3.7
18	R	16	PRO	3.7
1	A	1034	G	3.7
1	A	1035	A	3.6
1	A	1006(A)	C	3.6
6	F	14	LEU	3.6
3	C	64	VAL	3.5
4	D	26	CYS	3.5
2	B	188	ALA	3.5
1	A	1134	G	3.4
1	A	1442	G	3.4
20	T	105	SER	3.4
10	J	76	ASN	3.4
4	D	22	LYS	3.4
1	A	159	G	3.4
1	A	1421	G	3.4
10	J	93	GLY	3.3
1	A	1022	G	3.3
1	A	191	G	3.3
4	D	30	LYS	3.3
1	A	1018	C	3.3
1	A	96	G	3.3
3	C	79	ARG	3.3
3	C	80	GLY	3.2
1	A	1027	C	3.2
1	A	1143	G	3.2
1	A	474	G	3.2
1	A	1213	A	3.2
2	B	203	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
10	J	83	GLU	3.2
6	F	1	MET	3.1
7	G	70	LYS	3.1
2	B	125	PRO	3.1
4	D	24	GLU	3.1
1	A	1030(C)	G	3.1
1	A	1019	C	3.1
1	A	1474	G	3.1
10	J	9	ARG	3.1
20	T	101	GLY	3.0
1	A	1144	G	3.0
17	Q	15	MET	3.0
1	A	993	G	3.0
13	M	119	GLY	3.0
18	R	17	SER	3.0
1	A	1128	C	3.0
1	A	1140	C	3.0
3	C	78	GLY	3.0
1	A	97	G	3.0
1	A	841	U	2.9
3	C	67	THR	2.9
1	A	1259	C	2.9
1	A	1043	C	2.9
4	D	2	GLY	2.9
1	A	183	G	2.9
1	A	1030(A)	G	2.9
1	A	1025	U	2.8
3	C	81	GLY	2.8
1	A	1422	G	2.8
1	A	1008	C	2.8
20	T	44	ALA	2.8
1	A	161	A	2.8
2	B	35	GLU	2.8
1	A	1139	G	2.8
16	P	83	GLU	2.8
13	M	117	VAL	2.8
2	B	40	HIS	2.8
19	S	5	LEU	2.8
1	A	190	C	2.8
1	A	447	G	2.7
1	A	1132	C	2.7
13	M	100	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	102	ASN	2.7
2	B	83	MET	2.7
7	G	139	GLU	2.7
1	A	1013	G	2.7
9	I	4	TYR	2.7
10	J	25	GLU	2.7
10	J	79	ARG	2.7
7	G	48	LYS	2.7
1	A	992	U	2.7
17	Q	105	ALA	2.7
1	A	1030(B)	C	2.7
10	J	92	THR	2.7
19	S	3	ARG	2.7
20	T	106	ALA	2.7
1	A	1275	A	2.7
2	B	15	VAL	2.6
3	C	69	HIS	2.6
1	A	1531	A	2.6
3	C	65	ALA	2.6
2	B	131	PRO	2.6
17	Q	102	GLY	2.6
1	A	1283	G	2.5
9	I	65	VAL	2.5
1	A	1277	C	2.5
1	A	1459	C	2.5
20	T	92	LEU	2.5
3	C	98	ASN	2.5
1	A	1175	G	2.5
3	C	74	GLY	2.5
9	I	67	GLY	2.5
1	A	420	U	2.5
12	L	60	LEU	2.5
1	A	1127	G	2.5
1	A	196	A	2.5
19	S	47	HIS	2.5
1	A	1467	G	2.5
1	A	413	G	2.5
1	A	1137	C	2.4
2	B	233	SER	2.4
11	K	129	SER	2.4
3	C	100	ALA	2.4
18	R	20	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	33	MET	2.4
19	S	26	GLY	2.4
1	A	540	G	2.4
3	C	206	GLU	2.4
3	C	47	LEU	2.4
1	A	1037	C	2.4
1	A	1012	U	2.4
1	A	1443	G	2.4
18	R	25	THR	2.4
9	I	128	ARG	2.3
2	B	127	ILE	2.3
1	A	1141	C	2.3
19	S	34	TRP	2.3
1	A	181	G	2.3
3	C	125	GLU	2.3
1	A	1009	G	2.3
1	A	1482	G	2.3
6	F	24	GLU	2.3
1	A	344	A	2.3
1	A	1021	G	2.3
1	A	1271	G	2.3
3	C	20	SER	2.3
1	A	427	U	2.3
15	O	23	GLY	2.3
23	Y	40	U	2.3
9	I	97	LYS	2.3
13	M	37	THR	2.2
12	L	77	LEU	2.2
3	C	176	HIS	2.2
19	S	12	ASP	2.2
1	A	1418	A	2.2
1	A	1258	G	2.2
1	A	1423	G	2.2
7	G	125	MET	2.2
3	C	60	ALA	2.2
1	A	532	A	2.2
7	G	69	VAL	2.2
2	B	123	ALA	2.2
1	A	1210	C	2.2
1	A	1050	G	2.2
1	A	1533	C	2.1
1	A	1030(D)	A	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	71	ALA	2.1
4	D	32	ALA	2.1
14	N	2	ALA	2.1
11	K	37	GLY	2.1
2	B	122	PHE	2.1
1	A	1174	G	2.1
2	B	124	SER	2.1
1	A	494	G	2.1
14	N	30	ALA	2.1
1	A	848	C	2.1
3	C	105	GLU	2.1
10	J	77	PRO	2.1
3	C	89	GLU	2.0
13	M	8	GLU	2.0
19	S	23	ASN	2.0
1	A	343	U	2.0
14	N	4	LYS	2.0
1	A	1133	G	2.0
9	I	117	HIS	2.0
9	I	94	ALA	2.0
1	A	445	G	2.0
1	A	195	A	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	G	3002	1/1	0.06	1.42	84,84,84,84	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	G	3023	1/1	0.37	1.17	84,84,84,84	0
25	MG	G	3061	1/1	0.43	0.66	84,84,84,84	0
25	MG	G	3004	1/1	0.44	0.49	84,84,84,84	0
25	MG	G	3050	1/1	0.46	0.84	84,84,84,84	0
25	MG	G	3030	1/1	0.46	0.81	84,84,84,84	0
25	MG	G	3059	1/1	0.56	0.38	84,84,84,84	0
25	MG	G	3048	1/1	0.63	0.64	84,84,84,84	0
25	MG	G	3064	1/1	0.63	0.45	84,84,84,84	0
25	MG	G	3067	1/1	0.64	0.73	84,84,84,84	0
25	MG	G	3049	1/1	0.67	1.02	84,84,84,84	0
25	MG	G	3069	1/1	0.67	0.27	84,84,84,84	0
25	MG	G	3071	1/1	0.67	0.35	84,84,84,84	0
26	K	G	3077	1/1	0.69	0.87	84,84,84,84	1
26	K	G	3078	1/1	0.69	0.29	84,84,84,84	1
25	MG	G	3018	1/1	0.70	0.71	84,84,84,84	0
25	MG	G	3036	1/1	0.71	0.76	84,84,84,84	0
25	MG	G	3046	1/1	0.72	0.24	84,84,84,84	0
25	MG	G	3042	1/1	0.73	1.27	84,84,84,84	0
25	MG	G	3057	1/1	0.73	1.29	84,84,84,84	0
26	K	G	3075	1/1	0.74	0.54	84,84,84,84	1
25	MG	G	3040	1/1	0.75	0.98	84,84,84,84	0
25	MG	G	3007	1/1	0.75	1.19	84,84,84,84	0
25	MG	G	3035	1/1	0.76	0.50	84,84,84,84	0
25	MG	G	3054	1/1	0.76	0.43	84,84,84,84	0
25	MG	G	3037	1/1	0.77	0.54	84,84,84,84	0
25	MG	G	3005	1/1	0.78	1.02	84,84,84,84	0
25	MG	G	3047	1/1	0.78	0.75	84,84,84,84	0
25	MG	G	3017	1/1	0.79	0.45	84,84,84,84	0
25	MG	G	3058	1/1	0.80	0.60	84,84,84,84	0
25	MG	G	3010	1/1	0.80	1.13	84,84,84,84	0
25	MG	G	3070	1/1	0.83	0.28	84,84,84,84	0
25	MG	G	3041	1/1	0.83	0.57	84,84,84,84	0
25	MG	G	3060	1/1	0.83	0.52	84,84,84,84	0
25	MG	G	3068	1/1	0.83	0.69	84,84,84,84	0
25	MG	G	3034	1/1	0.83	0.47	84,84,84,84	0
25	MG	G	3066	1/1	0.84	0.64	84,84,84,84	0
25	MG	G	3033	1/1	0.84	1.15	84,84,84,84	0
25	MG	G	3020	1/1	0.84	0.74	84,84,84,84	0
25	MG	G	3044	1/1	0.85	1.05	84,84,84,84	0
25	MG	G	3031	1/1	0.85	0.28	84,84,84,84	0
26	K	G	3074	1/1	0.85	0.44	84,84,84,84	1

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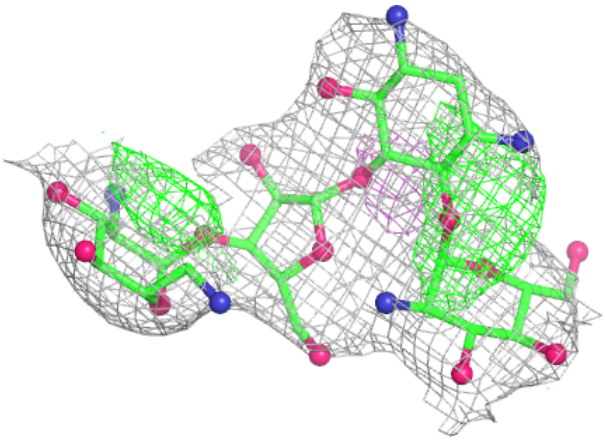
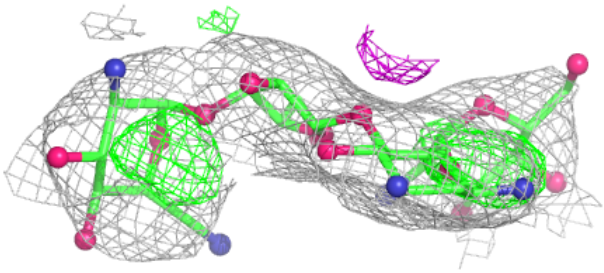
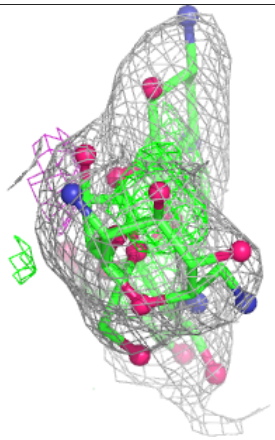
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	G	3014	1/1	0.85	1.18	84,84,84,84	0
25	MG	G	3006	1/1	0.85	0.71	84,84,84,84	0
25	MG	G	3062	1/1	0.85	0.70	84,84,84,84	0
26	K	G	3072	1/1	0.86	0.24	84,84,84,84	0
25	MG	G	3063	1/1	0.86	0.72	84,84,84,84	0
25	MG	G	3003	1/1	0.86	0.59	84,84,84,84	0
25	MG	G	3053	1/1	0.86	0.83	84,84,84,84	0
25	MG	G	3013	1/1	0.86	0.77	84,84,84,84	0
25	MG	G	3026	1/1	0.87	1.15	84,84,84,84	0
25	MG	G	3027	1/1	0.87	0.51	84,84,84,84	0
25	MG	G	3043	1/1	0.87	0.86	84,84,84,84	0
26	K	G	3076	1/1	0.88	0.13	84,84,84,84	0
26	K	G	3079	1/1	0.88	0.20	84,84,84,84	1
25	MG	G	3052	1/1	0.89	0.67	84,84,84,84	0
25	MG	G	3045	1/1	0.89	0.62	84,84,84,84	0
24	PAR	A	3001	42/42	0.89	0.28	84,84,84,84	0
25	MG	G	3028	1/1	0.89	0.97	84,84,84,84	0
25	MG	G	3056	1/1	0.90	0.64	84,84,84,84	0
25	MG	G	3025	1/1	0.90	0.65	84,84,84,84	0
25	MG	G	3024	1/1	0.91	0.73	84,84,84,84	0
25	MG	G	3029	1/1	0.91	1.17	84,84,84,84	0
25	MG	G	3009	1/1	0.91	0.15	84,84,84,84	0
25	MG	G	3065	1/1	0.92	0.13	84,84,84,84	0
25	MG	G	3015	1/1	0.92	0.61	84,84,84,84	0
25	MG	G	3016	1/1	0.93	0.69	84,84,84,84	0
26	K	G	3073	1/1	0.93	0.42	84,84,84,84	1
25	MG	G	3019	1/1	0.94	1.09	84,84,84,84	0
25	MG	G	3008	1/1	0.94	0.08	84,84,84,84	0
25	MG	G	3012	1/1	0.94	0.70	84,84,84,84	0
25	MG	G	3055	1/1	0.94	0.36	84,84,84,84	0
25	MG	G	3021	1/1	0.95	0.28	84,84,84,84	0
25	MG	G	3011	1/1	0.95	0.36	84,84,84,84	0
25	MG	G	3039	1/1	0.96	0.70	84,84,84,84	0
25	MG	G	3038	1/1	0.96	0.13	84,84,84,84	0
27	ZN	G	3080	1/1	0.96	0.26	84,84,84,84	1
25	MG	G	3051	1/1	0.97	0.63	84,84,84,84	0
25	MG	G	3022	1/1	0.98	0.39	84,84,84,84	0
25	MG	G	3032	1/1	0.98	1.23	84,84,84,84	0
27	ZN	G	3081	1/1	0.98	0.18	84,84,84,84	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 3001: 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 (i)

There are no such residues in this entry.