



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2014 – 06:08 PM BST

PDB ID : 4KD8  
Title : 70S Ribosome translocation intermediate FA-3.6A CONTAINING ELONGATION FACTOR EFG/FUSIDIC ACID/GDP, MRNA, AND TRNA BOUND IN THE  $pe^*/E$  STATE. THIS ENTRY CONTAINS THE 30S RIBOSOMAL SUBUNIT A. THE 50S SUBUNIT A CAN BE FOUND IN 4KD9. MOLECULE B IN THE SAME ASYMMETRIC UNIT IS DEPOSITED AS 4KDA (30S) AND 4KDB (50S).  
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.  
Deposited on : 2013-04-24  
Resolution : 3.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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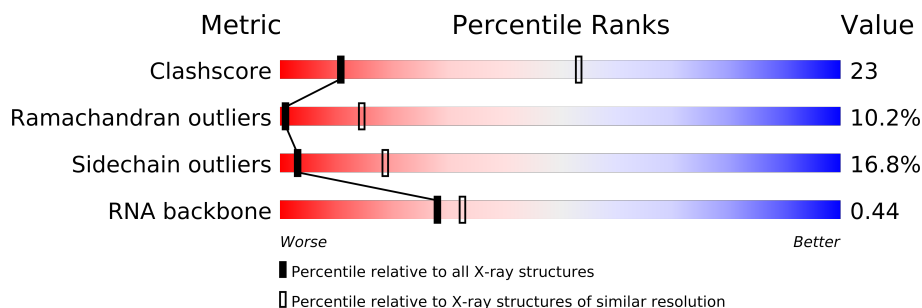
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	<b>FAILED</b>
EDS	:	<b>NOT EXECUTED</b>
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23004

# 1 Overall quality at a glance

The reported resolution of this entry is 3.50 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))
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RNA backbone	1838	1007 (4.22-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	235	
2	C	207	
3	D	208	
4	E	151	
5	F	101	
6	G	155	
7	H	138	
8	I	127	
9	J	99	
10	K	119	
11	L	125	
12	M	125	
13	N	60	
14	O	88	
15	P	84	

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Mol	Chain	Length	Quality of chain
16	Q	100	<div><div></div></div>
17	R	70	<div><div></div></div>
18	S	79	<div><div></div></div>
19	T	99	<div><div></div></div>
20	A	1511	<div><div></div></div>
21	W	77	<div><div></div></div>
22	V	23	<div><div></div></div>
23	Y	687	<div><div></div></div>
24	U	6	<div><div></div></div>

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 58959 atoms, of which 0 are hydrogen and 0 are deuterium.

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 protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	58	HIS	ARG	CONFLICT	UNP P62669

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

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

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Q	100	Total	C	N	O	S	0	0	0
			835	534	155	144	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLU	GLN	CONFLICT	UNP P62658

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	41	ILE	VAL	CONFLICT	UNP P62661

- Molecule 20 is a RNA chain called ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	A	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			

- Molecule 21 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	W	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			

- Molecule 22 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	667	Total	C	N	O	S	0	0	0
			5219	3318	893	990	18			

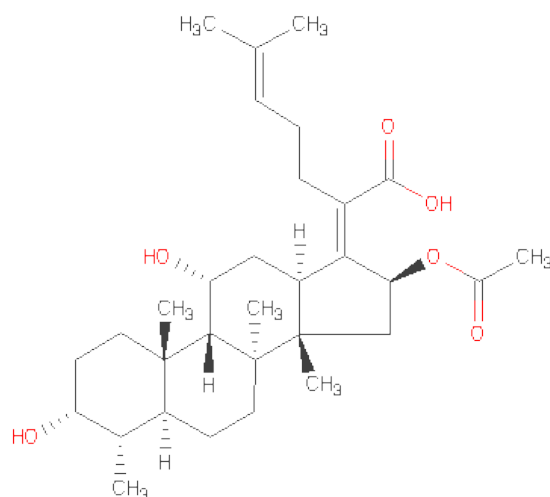
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	129	LYS	HIS	CONFLICT	UNP Q72I01
Y	226	ASN	HIS	CONFLICT	UNP Q72I01

- Molecule 24 is a protein called VIOMYCIN.

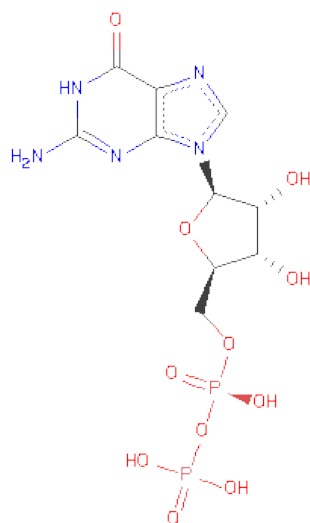
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	U	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 25 is FUSIDIC ACID (three-letter code: FUA) (formula:  $C_{31}H_{48}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	Y	1	Total	C	O	0	0
			37	31	6		

- Molecule 26 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	Y	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	Y	1	Total	Mg	0	0
			1	1		

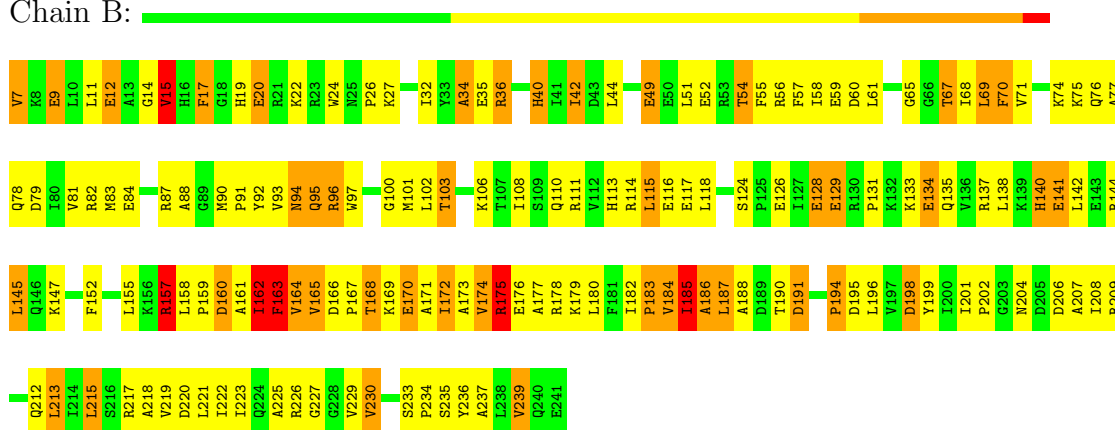
### 3 Residue-property plots

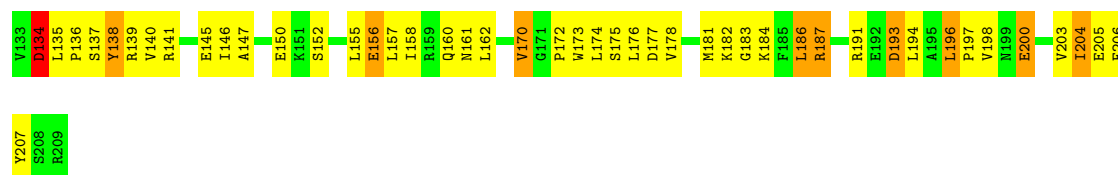
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: 30S ribosomal protein S2

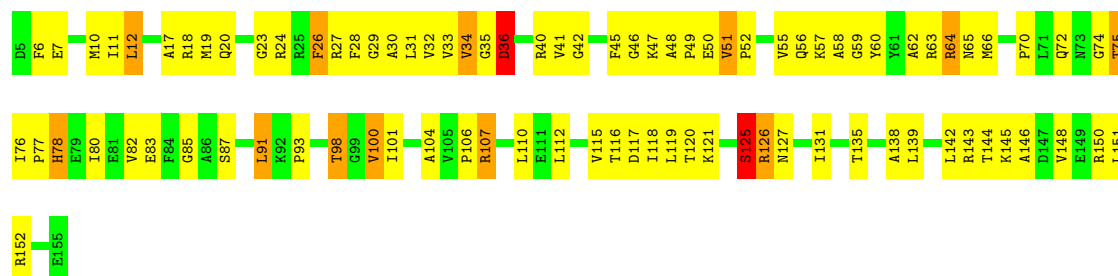
Chain B:





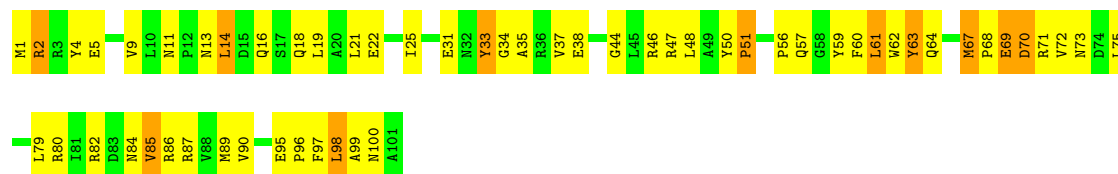
- Molecule 4: 30S ribosomal protein S5

Chain E:



- Molecule 5: 30S ribosomal protein S6

Chain F:



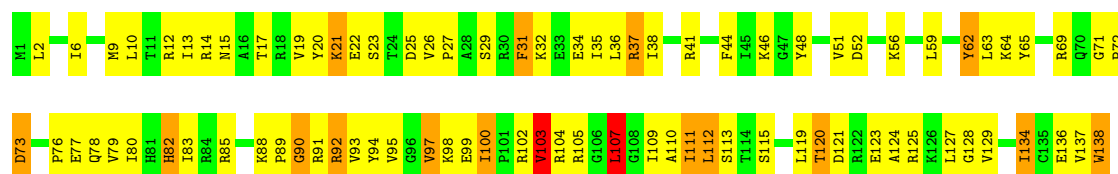
- Molecule 6: 30S ribosomal protein S7

Chain G:



- Molecule 7: 30S ribosomal protein S8

Chain H:



- Molecule 8: 30S ribosomal protein S9

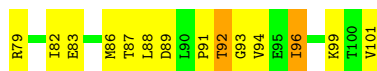
Chain I:





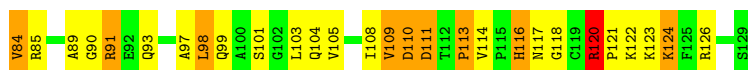
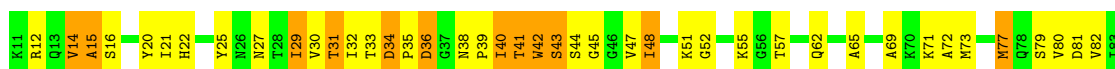
• Molecule 9: 30S ribosomal protein S10

Chain J:



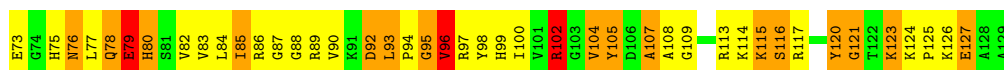
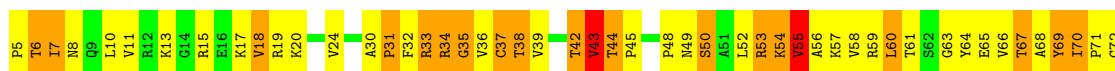
• Molecule 10: 30S ribosomal protein S11

Chain K:



• Molecule 11: 30S ribosomal protein S12

Chain L:



• Molecule 12: 30S ribosomal protein S13

Chain M:



• Molecule 13: 30S ribosomal protein S14 type Z

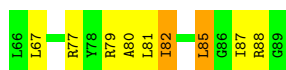
Chain N:



• Molecule 14: 30S ribosomal protein S15

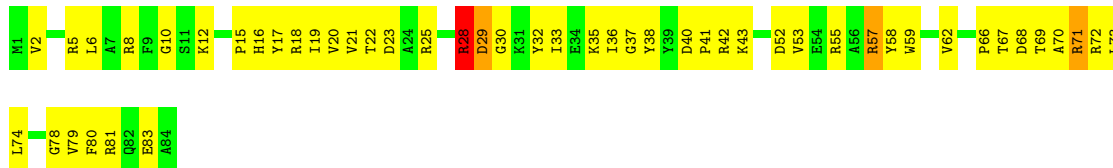
Chain O:





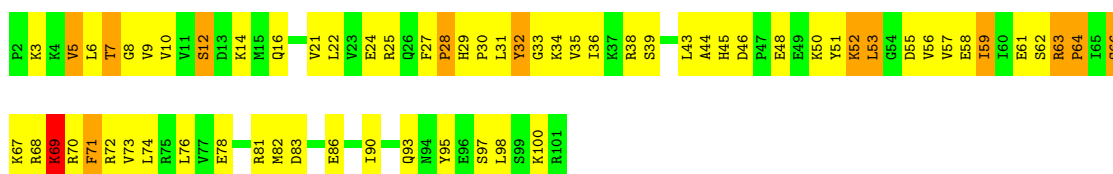
- Molecule 15: 30S ribosomal protein S16

Chain P:



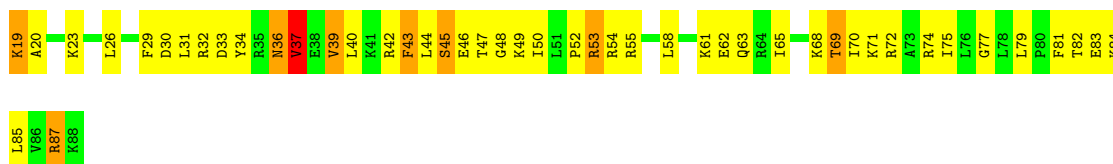
- Molecule 16: 30S ribosomal protein S17

Chain Q:



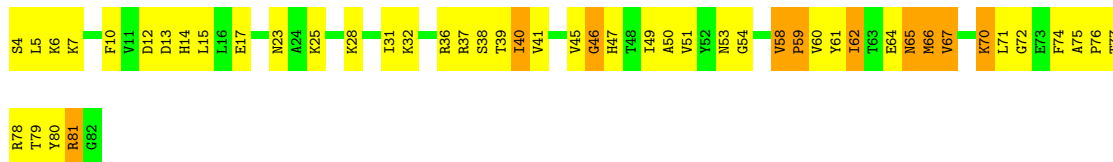
- Molecule 17: 30S ribosomal protein S18

Chain R:



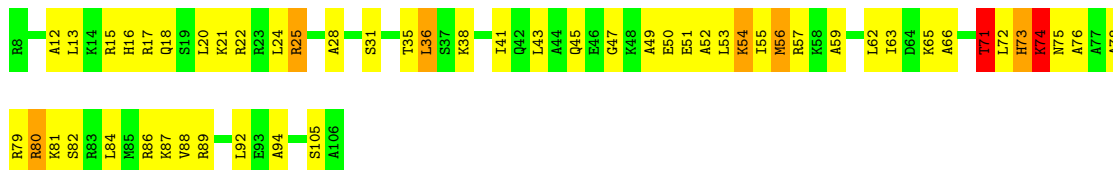
- Molecule 18: 30S ribosomal protein S19

Chain S:



- Molecule 19: 30S ribosomal protein S20

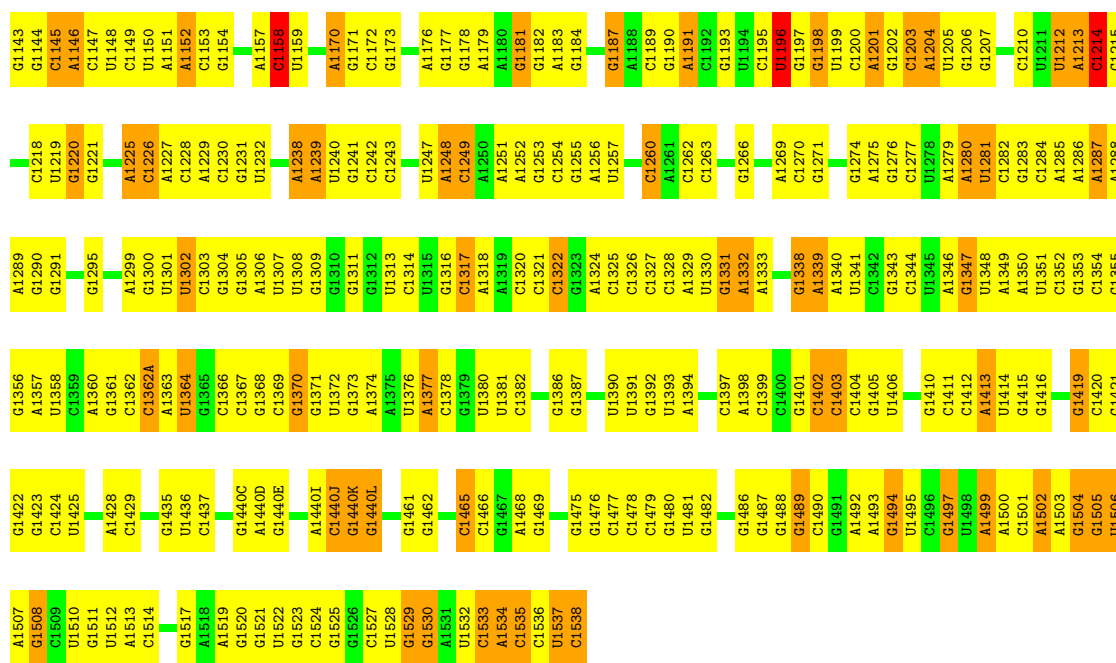
Chain T:



- Molecule 20: ribosomal RNA 16S

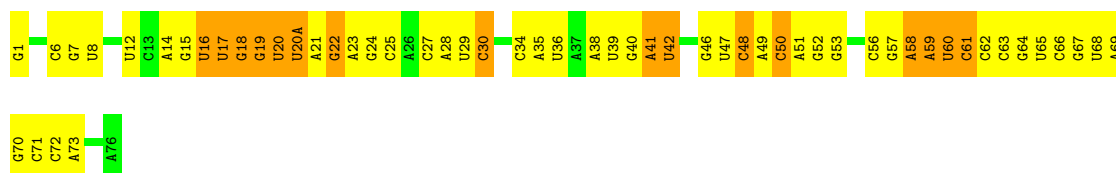
Chain A:





• Molecule 21: transfer RNA

Chain W:



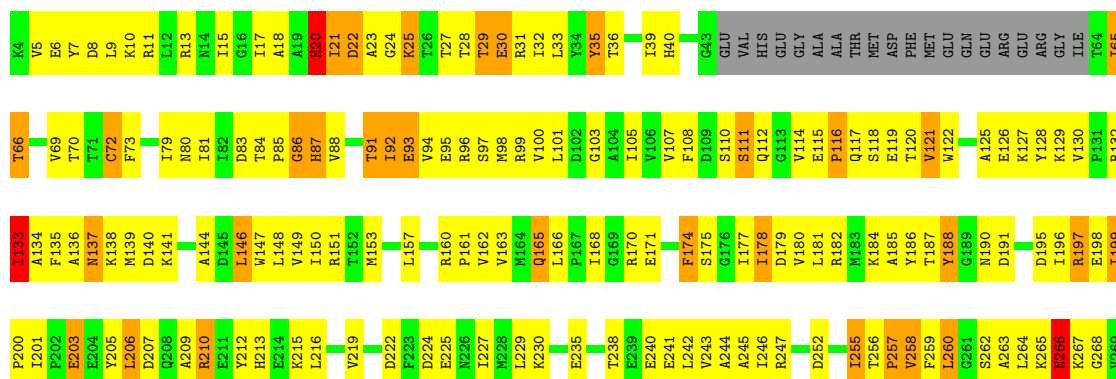
• Molecule 22: messenger RNA

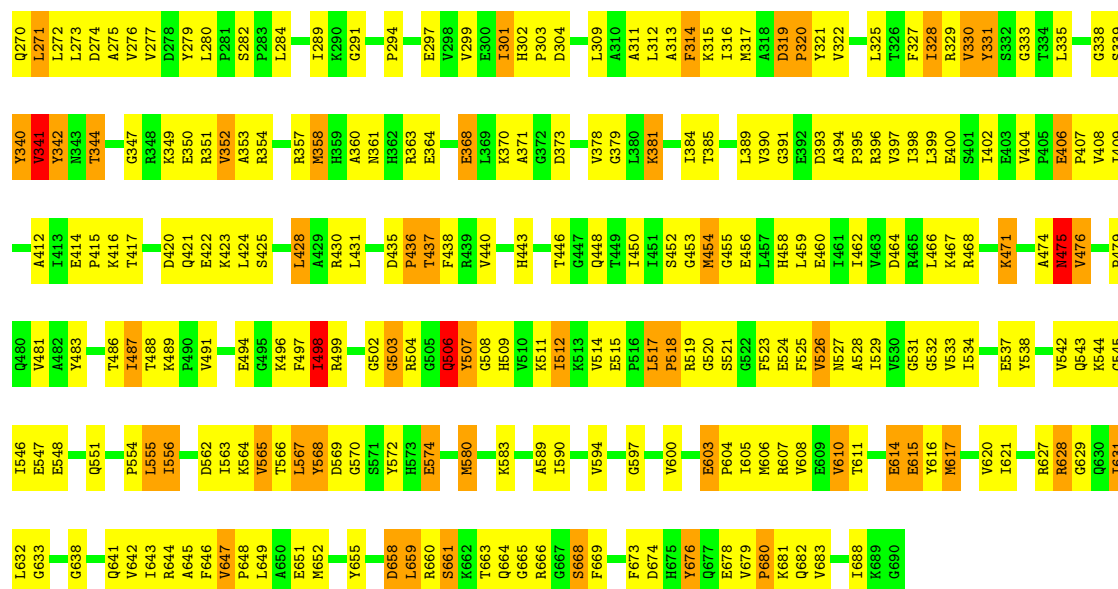
Chain V:



• Molecule 23: Elongation factor G

Chain Y:





• Molecule 24: VIOMYCIN

Chain U: 

There are no outlier residues recorded for this chain.



## 4 Data and refinement statistics

Xtriage (Phenix) failed to run properly; EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	308.96Å 670.66Å 347.77Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.284 , 0.328	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	58959	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, DPP, KBE, UAL, FUA, 5OH

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	B	0.38	0/1945	0.72	1/2621 (0.0%)
2	C	0.28	0/1645	0.53	0/2216
3	D	0.30	0/1733	0.58	0/2318
4	E	0.32	0/1172	0.58	1/1576 (0.1%)
5	F	0.31	0/856	0.59	0/1154
6	G	0.29	0/1276	0.51	0/1709
7	H	0.30	0/1136	0.57	0/1527
8	I	0.29	0/1029	0.53	0/1379
9	J	0.27	0/815	0.54	0/1095
10	K	0.33	0/900	0.61	0/1213
11	L	0.40	0/992	0.83	2/1327 (0.2%)
12	M	0.29	0/1008	0.59	1/1347 (0.1%)
13	N	0.30	0/501	0.52	0/664
14	O	0.31	0/745	0.52	0/992
15	P	0.28	0/722	0.50	0/970
16	Q	0.36	0/848	0.65	0/1131
17	R	0.31	0/579	0.59	0/768
18	S	0.31	0/647	0.60	0/870
19	T	0.33	0/765	0.56	0/1007
20	A	0.37	0/36351	1.02	61/56736 (0.1%)
21	W	0.33	0/1827	1.03	0/2845
22	V	0.27	0/568	0.81	0/886
23	Y	0.34	1/5317 (0.0%)	0.66	7/7198 (0.1%)
24	U	0.95	0/11	1.28	0/13
All	All	0.35	1/63388 (0.0%)	0.89	73/93562 (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	B	0	3
23	Y	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	506	GLN	C-N	-5.48	1.21	1.34

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	506	GLN	O-C-N	-12.49	102.72	122.70
20	A	815	A	C5-C6-N6	11.75	133.10	123.70
20	A	815	A	N1-C6-N6	-11.03	111.98	118.60
20	A	1508	G	N1-C2-N3	8.68	129.11	123.90
20	A	1158	C	C2-N1-C1'	8.16	127.78	118.80
20	A	838(C)	U	C2-N1-C1'	8.04	127.35	117.70
23	Y	502	GLY	CA-C-N	-7.95	100.30	116.20
23	Y	503	GLY	O-C-N	-7.83	110.17	122.70
23	Y	506	GLN	CA-C-N	7.81	134.39	117.20
20	A	815	A	N3-C4-N9	-7.71	121.23	127.40
20	A	1508	G	C2-N3-C4	-7.64	108.08	111.90
20	A	815	A	C6-N1-C2	7.53	123.12	118.60
20	A	1158	C	N1-C2-O2	7.46	123.38	118.90
20	A	815	A	N9-C4-C5	7.30	108.72	105.80
23	Y	506	GLN	C-N-CA	7.28	139.91	121.70
1	B	163	PHE	N-CA-C	-7.20	91.55	111.00
23	Y	502	GLY	O-C-N	7.18	135.41	123.20
20	A	1170	A	N1-C6-N6	7.07	122.84	118.60
20	A	838(C)	U	N1-C2-O2	7.07	127.75	122.80
20	A	421	U	C2-N1-C1'	6.95	126.03	117.70
20	A	815	A	C6-C5-N7	6.89	137.12	132.30
20	A	754	C	C2-N1-C1'	6.85	126.33	118.80
20	A	838(C)	U	N3-C2-O2	-6.63	117.56	122.20
20	A	618	C	C6-N1-C1'	6.62	128.75	120.80
20	A	618	C	C5-C4-N4	6.40	124.68	120.20
20	A	717	C	C2-N1-C1'	6.30	125.74	118.80
20	A	1158	C	C6-N1-C1'	-6.22	113.33	120.80
4	E	12	LEU	CA-CB-CG	6.18	129.51	115.30
20	A	421	U	N1-C2-O2	6.15	127.11	122.80
20	A	68(R)	C	N1-C2-O2	-6.12	115.23	118.90
20	A	618	C	O4'-C1'-N1	6.03	113.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	383	A	N1-C6-N6	6.02	122.21	118.60
20	A	1066	C	C2-N1-C1'	6.00	125.40	118.80
20	A	1158	C	N3-C2-O2	-5.99	117.71	121.90
12	M	56	LEU	CA-CB-CG	5.99	129.06	115.30
20	A	1332	A	N1-C6-N6	5.87	122.12	118.60
20	A	618	C	N3-C4-C5	-5.87	119.55	121.90
20	A	618	C	C2-N1-C1'	-5.86	112.35	118.80
20	A	129(A)	G	N3-C2-N2	5.84	123.99	119.90
20	A	1043	C	O4'-C1'-N1	5.81	112.85	108.20
20	A	1214	C	C2-N1-C1'	5.80	125.18	118.80
20	A	1214	C	N1-C2-O2	5.71	122.32	118.90
20	A	960	U	N1-C2-O2	5.63	126.74	122.80
20	A	1170	A	C4-C5-C6	5.62	119.81	117.00
20	A	186(G)	C	C6-N1-C2	-5.61	118.06	120.30
20	A	717	C	C6-N1-C1'	-5.60	114.08	120.80
20	A	68(H)	G	C8-N9-C4	-5.59	104.17	106.40
20	A	815	A	C5-C6-N1	-5.58	114.91	117.70
20	A	68(R)	C	C2-N1-C1'	-5.57	112.67	118.80
20	A	1465	C	C2-N3-C4	-5.55	117.12	119.90
20	A	68(H)	G	N9-C4-C5	5.53	107.61	105.40
20	A	748	C	P-O3'-C3'	5.51	126.31	119.70
20	A	68(R)	C	C6-N1-C1'	5.51	127.41	120.80
20	A	1508	G	C6-C5-N7	-5.49	127.10	130.40
11	L	55	VAL	CB-CA-C	-5.43	101.08	111.40
20	A	943	U	C5-C4-O4	5.42	129.15	125.90
20	A	1196	U	C2-N1-C1'	5.41	124.19	117.70
20	A	383	A	C4-C5-C6	5.36	119.68	117.00
20	A	1071	C	C5-C6-N1	5.34	123.67	121.00
20	A	186(G)	C	N3-C2-O2	-5.33	118.17	121.90
20	A	421	U	N3-C2-O2	-5.22	118.55	122.20
20	A	320	C	O4'-C1'-N1	5.22	112.37	108.20
20	A	838(C)	U	C6-N1-C1'	-5.21	113.90	121.20
20	A	1465	C	C5-C4-N4	-5.17	116.58	120.20
20	A	717	C	N1-C2-O2	5.16	121.99	118.90
20	A	1066	C	C6-N1-C1'	-5.13	114.65	120.80
20	A	1101	A	P-O3'-C3'	5.12	125.85	119.70
20	A	1170	A	C6-C5-N7	-5.12	128.71	132.30
20	A	754	C	C6-N1-C2	-5.09	118.27	120.30
11	L	60	LEU	CA-CB-CG	5.08	126.99	115.30
20	A	129(A)	G	N9-C4-C5	-5.08	103.37	105.40
23	Y	502	GLY	C-N-CA	-5.05	111.69	122.30
20	A	1248	A	N1-C6-N6	-5.00	115.60	118.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	162	ILE	Peptide
1	B	170	GLU	Peptide
1	B	185	ILE	Peptide
23	Y	133	ILE	Peptide
23	Y	503	GLY	Mainchain
23	Y	506	GLN	Mainchain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1910	0	1957	135	0
2	C	1621	0	1688	87	0
3	D	1703	0	1763	104	0
4	E	1156	0	1213	70	0
5	F	843	0	857	42	0
6	G	1257	0	1296	54	0
7	H	1116	0	1177	67	0
8	I	1010	0	1037	78	0
9	J	802	0	849	44	0
10	K	885	0	904	54	0
11	L	976	0	1062	113	0
12	M	997	0	1072	67	0
13	N	492	0	529	37	0
14	O	734	0	771	47	0
15	P	706	0	725	45	0
16	Q	835	0	904	64	0
17	R	574	0	644	36	0
18	S	634	0	655	34	0
19	T	763	0	861	38	0
20	A	32474	0	16393	994	0
21	W	1635	0	831	60	0
22	V	503	0	252	12	0
23	Y	5219	0	5290	313	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	U	48	0	39	0	0
25	Y	37	0	47	6	0
26	Y	28	0	12	12	0
27	Y	1	0	0	0	0
All	All	58959	0	42828	2304	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (2304) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:W:15:G:N2	21:W:48:C:H42	1.36	1.24
21:W:15:G:H22	21:W:48:C:N4	1.38	1.21
20:A:815:A:N1	20:A:1508:G:N2	1.93	1.15
20:A:815:A:H2	20:A:1527:C:O2	1.29	1.15
21:W:50:C:N4	21:W:64:G:H1	1.50	1.08
20:A:1413:A:N6	20:A:1487:G:H1	1.53	1.05
20:A:815:A:C2	20:A:1527:C:O2	2.13	0.99
23:Y:137:ASN:HD22	23:Y:138:LYS:H	1.11	0.94
20:A:112:G:H1	20:A:315:A:H61	1.07	0.92
11:L:56:ALA:HB3	11:L:68:ALA:HB3	1.52	0.91
23:Y:137:ASN:HD21	23:Y:263:ALA:H	1.06	0.90
23:Y:137:ASN:ND2	23:Y:138:LYS:H	1.70	0.90
6:G:79:ARG:HB3	20:A:1381:U:H1'	1.54	0.89
20:A:68(E):G:O6	20:A:68(U):U:O2	1.90	0.88
11:L:58:VAL:HG12	11:L:60:LEU:H	1.36	0.88
11:L:35:GLY:HA2	11:L:58:VAL:HG13	1.56	0.88
3:D:23:GLY:HA3	3:D:112:VAL:HG22	1.53	0.88
3:D:102:ASP:HA	3:D:121:VAL:HG21	1.53	0.87
21:W:53:G:H1	21:W:61:C:H42	1.18	0.85
20:A:687:A:H62	20:A:703:G:H21	1.24	0.85
21:W:18:G:N2	21:W:58:A:OP1	2.10	0.84
8:I:2:GLU:N	8:I:88:TYR:HH	1.74	0.84
20:A:406:G:H1	20:A:436:C:H42	1.23	0.84
23:Y:85:PRO:HB3	23:Y:94:VAL:HA	1.59	0.84
21:W:50:C:H42	21:W:64:G:H1	0.89	0.84
20:A:977:A:HO2'	20:A:981:U:H3	1.22	0.84
8:I:4:TYR:HB2	8:I:19:LEU:HB2	1.58	0.83
20:A:1510:U:H3	20:A:1525:G:H1	1.25	0.83
20:A:1077:G:N2	20:A:1080:A:OP2	2.11	0.83
20:A:681:C:H42	20:A:709:G:H1	1.26	0.82
3:D:3:ARG:HH22	3:D:5:ILE:HD12	1.45	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1065:U:O2	20:A:1067:A:N6	2.12	0.82
2:C:54:ARG:HB2	2:C:69:HIS:HB2	1.60	0.82
2:C:88:ARG:HH21	2:C:100:ALA:HA	1.44	0.82
14:O:39:LEU:HD12	14:O:56:LEU:HB2	1.62	0.82
20:A:961:U:O2	20:A:1201:A:N1	2.13	0.82
23:Y:633:GLY:HA3	23:Y:644:ARG:HB2	1.63	0.81
2:C:50:ALA:HB1	2:C:72:LYS:HB3	1.62	0.81
20:A:1528:U:H4'	20:A:1529:G:H21	1.43	0.81
1:B:69:LEU:HB3	1:B:162:ILE:HG22	1.62	0.81
23:Y:137:ASN:HD22	23:Y:138:LYS:N	1.78	0.80
20:A:296:U:H3	20:A:301:G:H1	1.28	0.80
23:Y:137:ASN:HD21	23:Y:263:ALA:N	1.79	0.80
3:D:57:ARG:HH21	4:E:107:ARG:HH21	1.28	0.80
20:A:908:A:H2'	20:A:909:A:C8	2.17	0.80
20:A:112:G:H1	20:A:315:A:N6	1.80	0.80
23:Y:201:ILE:HG12	23:Y:206:LEU:H	1.46	0.80
20:A:1003:G:N1	20:A:1037:C:O2	2.15	0.79
11:L:71:PRO:O	11:L:102:ARG:NH1	2.16	0.79
11:L:71:PRO:HB2	11:L:102:ARG:HH11	1.48	0.79
11:L:89:ARG:HA	11:L:96:VAL:HB	1.65	0.79
14:O:39:LEU:HD23	20:A:740:U:H4'	1.63	0.78
3:D:175:SER:HB3	3:D:184:LYS:HB2	1.65	0.78
23:Y:497:PHE:HB3	23:Y:508:GLY:H	1.49	0.78
23:Y:137:ASN:ND2	26:Y:702:GDP:O6	2.17	0.78
1:B:204:ASN:OD1	1:B:207:ALA:N	2.15	0.78
23:Y:133:ILE:HD12	23:Y:280:LEU:HD21	1.65	0.78
23:Y:607:ARG:HG3	23:Y:674:ASP:HB2	1.67	0.77
20:A:107:G:OP1	20:A:325:A:N6	2.17	0.77
23:Y:608:VAL:HG21	23:Y:652:MET:HE2	1.67	0.77
14:O:39:LEU:HD21	14:O:52:SER:HB3	1.66	0.77
20:A:285:G:H2'	20:A:286:G:H8	1.50	0.77
23:Y:230:LYS:HG3	23:Y:235:GLU:HB3	1.65	0.77
23:Y:517:LEU:HG	23:Y:518:PRO:HD2	1.65	0.76
1:B:84:GLU:HB3	1:B:219:VAL:HG21	1.67	0.76
20:A:1505:G:H5''	20:A:1506:U:H5''	1.66	0.76
4:E:125:SER:OG	20:A:19:C:OP1	2.04	0.76
14:O:23:GLY:O	20:A:750:G:N2	2.18	0.76
20:A:1060:C:H2'	20:A:1061:G:H8	1.50	0.76
1:B:167:PRO:O	1:B:171:ALA:HB2	1.84	0.76
3:D:122:ARG:HE	20:A:403:C:H4'	1.50	0.76
23:Y:566:THR:HG22	23:Y:567:LEU:H	1.50	0.76
20:A:973:G:H3'	20:A:974:A:H5''	1.67	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:441:A:H62	20:A:493:G:H21	1.33	0.75
20:A:559:A:H4'	20:A:560:U:H5''	1.68	0.75
16:Q:28:PRO:HA	16:Q:35:VAL:HA	1.66	0.75
2:C:67:THR:HA	2:C:102:ASN:HB3	1.66	0.75
3:D:68:TYR:O	3:D:70:ILE:N	2.18	0.75
1:B:19:HIS:HB2	1:B:204:ASN:HD22	1.52	0.75
20:A:713:G:H2'	20:A:714:G:C8	2.21	0.75
10:K:32:ILE:HD13	10:K:72:ALA:HB2	1.69	0.75
23:Y:314:PHE:HZ	23:Y:329:ARG:HB3	1.51	0.75
20:A:585:G:H1	20:A:756:C:H42	1.33	0.74
20:A:1065:U:H4'	20:A:1066:C:H5''	1.69	0.74
2:C:5:ILE:HG21	20:A:1189:C:H5''	1.67	0.74
10:K:22:HIS:HB3	10:K:29:ILE:HG22	1.70	0.74
20:A:1281:U:H5'	20:A:1282:C:H5	1.52	0.74
11:L:52:LEU:H	11:L:53:ARG:HD2	1.52	0.74
20:A:673:G:H2'	20:A:674:G:C8	2.23	0.74
21:W:15:G:N1	21:W:48:C:N3	2.30	0.74
1:B:171:ALA:HA	1:B:174:VAL:HB	1.67	0.74
17:R:52:PRO:HB3	20:A:720:C:H5''	1.70	0.74
20:A:33:A:H2	20:A:551:U:H3	1.35	0.74
6:G:87:VAL:HG22	6:G:151:TYR:HB3	1.68	0.74
2:C:48:TYR:O	2:C:50:ALA:N	2.21	0.74
10:K:29:ILE:HD11	10:K:42:TRP:HB2	1.70	0.74
12:M:120:LYS:HG2	20:A:955:U:H5'	1.69	0.74
23:Y:428:LEU:HA	23:Y:431:LEU:HB2	1.70	0.74
6:G:78:ARG:HB3	6:G:85:TYR:HB2	1.69	0.74
23:Y:72:CYS:HB3	23:Y:79:ILE:HB	1.70	0.74
2:C:102:ASN:HD21	2:C:104:GLN:HG2	1.53	0.73
3:D:187:ARG:NH2	3:D:193:ASP:OD2	2.21	0.73
1:B:162:ILE:HB	1:B:164:VAL:HG23	1.70	0.73
19:T:86:ARG:NH2	20:A:258:G:OP1	2.20	0.73
10:K:99:GLN:HG2	10:K:105:VAL:HG21	1.69	0.73
14:O:38:ARG:HH11	14:O:38:ARG:HA	1.52	0.73
1:B:204:ASN:HD21	1:B:206:ASP:HB2	1.53	0.73
12:M:115:LYS:NZ	20:A:1228:C:OP1	2.22	0.73
16:Q:10:VAL:HA	16:Q:21:VAL:HG22	1.70	0.73
20:A:1135:U:O2	20:A:1138:G:N2	2.20	0.73
1:B:174:VAL:HG22	1:B:184:VAL:HG11	1.70	0.73
21:W:15:G:H22	21:W:48:C:H42	0.75	0.73
8:I:120:ARG:HD2	20:A:1348:U:H4'	1.68	0.73
11:L:85:ILE:HG23	11:L:98:TYR:HB3	1.70	0.72
23:Y:408:VAL:HG22	23:Y:454:MET:HA	1.69	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:N:41:ARG:HH22	20:A:973:G:H4'	1.53	0.72
1:B:35:GLU:HA	1:B:40:HIS:HA	1.71	0.72
1:B:170:GLU:O	1:B:174:VAL:HG23	1.89	0.72
20:A:1060:C:H2'	20:A:1061:G:C8	2.25	0.72
20:A:505:G:H1	20:A:526:C:H42	1.36	0.72
9:J:16:LEU:HD11	9:J:70:ARG:HD3	1.71	0.72
10:K:33:THR:HA	10:K:39:PRO:HA	1.72	0.72
20:A:975:A:H4'	20:A:976:G:H5''	1.69	0.72
16:Q:43:LEU:HD12	16:Q:69:LYS:HA	1.71	0.72
23:Y:603:GLU:OE2	23:Y:628:ARG:NH2	2.22	0.72
23:Y:276:VAL:HA	23:Y:280:LEU:HD23	1.71	0.72
12:M:114:ARG:HB3	20:A:1228:C:H5''	1.72	0.71
11:L:53:ARG:HG2	11:L:93:LEU:HD22	1.72	0.71
20:A:1502:A:H8	20:A:1505:G:H22	1.38	0.71
10:K:21:ILE:HB	10:K:84:VAL:HA	1.71	0.71
15:P:30:GLY:HA2	20:A:309:G:H5''	1.72	0.71
12:M:99:ARG:NH2	20:A:1308:U:OP2	2.24	0.71
4:E:148:VAL:HG13	4:E:152:ARG:HD2	1.73	0.71
20:A:427:U:H4'	20:A:541:G:H5''	1.71	0.71
20:A:1414:U:H2'	20:A:1415:G:H8	1.56	0.71
2:C:157:ILE:HD13	2:C:164:ARG:HE	1.56	0.71
6:G:57:GLU:HB2	6:G:60:LYS:HB2	1.71	0.71
11:L:124:LYS:NZ	20:A:501:C:OP2	2.20	0.71
4:E:18:ARG:NH2	20:A:1070:U:OP1	2.24	0.71
18:S:39:THR:HA	18:S:70:LYS:HA	1.71	0.70
11:L:92:ASP:OD1	11:L:92:ASP:N	2.24	0.70
8:I:21:PRO:HA	8:I:59:PHE:HA	1.73	0.70
25:Y:701:FUA:H5	25:Y:701:FUA:H202	1.73	0.70
23:Y:341:VAL:HG12	23:Y:391:GLY:HA2	1.74	0.70
20:A:373:A:N3	20:A:481:G:N2	2.35	0.70
20:A:28:G:O2'	20:A:296:U:OP1	2.09	0.70
10:K:40:ILE:HD13	20:A:685:G:H5'	1.73	0.70
20:A:367:U:H4'	23:Y:351:ARG:HE	1.55	0.70
20:A:801:U:H2'	20:A:802:A:H8	1.56	0.70
20:A:112:G:N2	20:A:315:A:N1	2.35	0.70
21:W:53:G:H1	21:W:61:C:N4	1.89	0.70
23:Y:315:LYS:HB3	23:Y:327:PHE:HD2	1.56	0.70
17:R:34:TYR:HB3	17:R:69:THR:HG22	1.73	0.70
12:M:105:THR:OG1	12:M:106:ASN:N	2.22	0.70
11:L:93:LEU:O	11:L:95:GLY:N	2.25	0.69
3:D:19:LEU:HB3	3:D:67:ILE:HD13	1.73	0.69
1:B:101:MET:HB2	1:B:102:LEU:HD12	1.73	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:L:42:THR:HA	11:L:52:LEU:HA	1.74	0.69
20:A:946:A:H2'	20:A:947:G:C8	2.26	0.69
20:A:940:C:H2'	20:A:941:G:C8	2.27	0.69
2:C:66:VAL:HB	2:C:101:LEU:HA	1.73	0.69
10:K:84:VAL:HG21	10:K:91:ARG:HD3	1.73	0.69
2:C:4:LYS:HE3	20:A:1191:A:H5'	1.74	0.69
17:R:26:LEU:HD11	17:R:42:ARG:HD2	1.75	0.69
11:L:37:CYS:SG	11:L:38:THR:N	2.65	0.69
20:A:1356:G:H2'	20:A:1357:A:C8	2.28	0.69
18:S:36:ARG:NH2	18:S:72:GLY:O	2.26	0.69
12:M:122:LYS:HB3	20:A:953:G:O2'	1.91	0.69
20:A:1321:C:H3'	20:A:1322:C:H5''	1.75	0.68
10:K:114:VAL:HG11	17:R:82:THR:HG21	1.74	0.68
20:A:697:U:O2	20:A:785:G:N2	2.26	0.68
20:A:1503:A:H61	22:V:14:A:H3'	1.57	0.68
21:W:66:C:H2'	21:W:67:G:H8	1.56	0.68
20:A:628:G:H2'	20:A:629:G:C8	2.28	0.68
20:A:114:U:O4	20:A:313:A:N1	2.26	0.68
1:B:88:ALA:HB1	1:B:222:ILE:HD11	1.75	0.68
23:Y:514:VAL:HA	23:Y:565:VAL:O	1.92	0.68
20:A:1440(J):C:O2'	20:A:1440(K):G:N3	2.27	0.68
20:A:612:C:H2'	20:A:613:C:C6	2.29	0.68
20:A:537:G:H2'	20:A:538:G:H8	1.59	0.68
1:B:34:ALA:HB1	1:B:36:ARG:HD2	1.75	0.68
3:D:20:TYR:O	3:D:22:LYS:N	2.27	0.68
20:A:537:G:H2'	20:A:538:G:C8	2.28	0.68
12:M:8:GLU:HG2	12:M:22:ILE:HG12	1.75	0.68
5:F:4:TYR:OH	20:A:738:C:OP1	2.11	0.68
23:Y:133:ILE:HG13	23:Y:272:LEU:HD11	1.75	0.68
18:S:78:ARG:O	18:S:81:ARG:NH1	2.27	0.68
23:Y:91:THR:O	23:Y:93:GLU:N	2.27	0.68
4:E:126:ARG:HE	20:A:9:G:H5''	1.59	0.68
12:M:58:GLU:O	12:M:62:ASN:ND2	2.26	0.68
1:B:27:LYS:HB2	1:B:194:PRO:HG3	1.76	0.68
23:Y:162:VAL:HB	23:Y:255:ILE:HG13	1.76	0.68
10:K:111:ASP:HA	17:R:84:LYS:HG3	1.75	0.67
20:A:68(B):G:O6	20:A:68(X):U:O2	2.12	0.67
21:W:12:U:H3	21:W:23:A:H61	1.42	0.67
16:Q:68:ARG:O	16:Q:70:ARG:N	2.26	0.67
23:Y:341:VAL:HG22	23:Y:352:VAL:HG12	1.74	0.67
18:S:36:ARG:HB2	18:S:72:GLY:HA3	1.77	0.67
20:A:520:A:H62	20:A:529:G:H21	1.42	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:J:51:ARG:HB3	20:A:1060:C:H4'	1.75	0.67
11:L:6:THR:O	11:L:8:ASN:N	2.28	0.67
20:A:68(E):G:C6	20:A:68(U):U:O2	2.47	0.67
8:I:113:LYS:H	8:I:119:ALA:HA	1.60	0.67
14:O:77:ARG:HA	14:O:80:ALA:HB3	1.76	0.67
14:O:16:ALA:HB1	14:O:21:ASP:HB3	1.76	0.67
20:A:68(F):C:H2'	20:A:68(G):G:C8	2.30	0.67
11:L:71:PRO:HG2	11:L:102:ARG:HG2	1.77	0.67
23:Y:679:VAL:HB	23:Y:683:VAL:HB	1.76	0.67
11:L:34:ARG:HG3	11:L:82:VAL:HG13	1.77	0.67
20:A:68(K):U:N3	20:A:68(N):U:OP2	2.26	0.67
21:W:50:C:N3	21:W:64:G:N2	2.38	0.67
11:L:70:ILE:HA	11:L:100:ILE:HB	1.76	0.66
16:Q:66:SER:OG	16:Q:67:LYS:N	2.27	0.66
2:C:8:ILE:HD11	2:C:184:TYR:HB3	1.77	0.66
20:A:458(A):G:H21	20:A:458(E):A:H62	1.43	0.66
12:M:37:THR:HG22	12:M:59:TYR:HB3	1.77	0.66
1:B:175:ARG:NH2	20:A:1075:C:O3'	2.27	0.66
1:B:95:GLN:OE1	1:B:96:ARG:NH1	2.29	0.66
16:Q:100:LYS:HB2	20:A:246:A:H3'	1.78	0.66
23:Y:22:ASP:O	26:Y:702:GDP:O3A	2.13	0.66
11:L:92:ASP:HB2	11:L:93:LEU:HD23	1.78	0.66
20:A:67:C:H2'	20:A:68:G:C8	2.30	0.66
20:A:1512:U:H2'	20:A:1513:A:C8	2.29	0.66
8:I:96:LEU:HG	8:I:101:PHE:HB2	1.78	0.66
20:A:237:C:H2'	20:A:238:G:C8	2.30	0.66
11:L:58:VAL:HG11	11:L:85:ILE:HG12	1.76	0.66
20:A:791:G:N2	20:A:1497:G:O3'	2.29	0.66
20:A:867:G:O2'	20:A:873:A:N1	2.28	0.66
3:D:101:LEU:HD11	3:D:126:ILE:HG21	1.78	0.66
20:A:681:C:N4	20:A:709:G:H1	1.94	0.66
21:W:39:U:H2'	21:W:40:G:H8	1.60	0.66
23:Y:631:ILE:HA	23:Y:645:ALA:HA	1.78	0.65
3:D:108:LEU:HD21	3:D:183:GLY:HA3	1.78	0.65
23:Y:24:GLY:C	26:Y:702:GDP:O2A	2.34	0.65
20:A:1308:U:H2'	20:A:1309:G:C8	2.31	0.65
23:Y:610:VAL:HG22	23:Y:643:ILE:HB	1.78	0.65
23:Y:256:THR:O	23:Y:258:VAL:N	2.29	0.65
23:Y:15:ILE:HD11	23:Y:81:ILE:HG13	1.77	0.65
20:A:34:C:H2'	20:A:35:G:C8	2.31	0.65
8:I:57:GLY:O	8:I:59:PHE:N	2.25	0.65
3:D:43:HIS:HA	3:D:46:LYS:HD3	1.78	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:152:SER:HA	3:D:155:LEU:HG	1.78	0.65
20:A:285:G:H2'	20:A:286:G:C8	2.32	0.65
21:W:66:C:H2'	21:W:67:G:C8	2.31	0.65
20:A:1391:U:H2'	20:A:1392:G:C8	2.32	0.64
20:A:418:C:H42	20:A:425:G:H1	1.45	0.64
17:R:40:LEU:HA	17:R:43:PHE:HB2	1.77	0.64
19:T:80:ARG:NH2	20:A:261:U:OP2	2.30	0.64
2:C:153:VAL:HG23	2:C:166:GLU:HB3	1.77	0.64
12:M:103:THR:HB	20:A:1226:C:H2'	1.80	0.64
8:I:127:LYS:HA	20:A:967:C:H5'	1.78	0.64
16:Q:62:SER:HB3	20:A:186(I):U:H3	1.61	0.64
20:A:663:A:H61	20:A:742:G:H1	1.44	0.64
20:A:1413:A:N1	20:A:1487:G:N2	2.32	0.64
23:Y:335:LEU:HD11	23:Y:352:VAL:HG11	1.79	0.64
16:Q:45:HIS:HB3	16:Q:72:ARG:HA	1.78	0.64
9:J:40:LEU:HD22	9:J:41:PRO:HD2	1.79	0.64
15:P:57:ARG:NH2	15:P:78:GLY:O	2.31	0.64
14:O:23:GLY:H	14:O:27:VAL:HG21	1.63	0.64
5:F:98:LEU:HB3	17:R:30:ASP:HA	1.80	0.64
9:J:65:LEU:HA	13:N:56:VAL:HA	1.79	0.64
23:Y:137:ASN:ND2	23:Y:262:SER:HA	2.13	0.64
1:B:58:ILE:HD11	1:B:185:ILE:HG21	1.79	0.64
23:Y:315:LYS:HB3	23:Y:327:PHE:CD2	2.32	0.64
1:B:175:ARG:HH22	20:A:1076:C:H5'	1.62	0.64
6:G:95:ARG:HH22	20:A:938:A:H4'	1.63	0.64
10:K:34:ASP:O	10:K:36:ASP:N	2.30	0.64
20:A:1015:A:H2'	20:A:1016:A:C8	2.33	0.64
20:A:599:C:H42	20:A:639:G:H1	1.46	0.64
6:G:75:VAL:HA	6:G:88:PRO:HA	1.78	0.64
3:D:107:ARG:HB3	3:D:174:LEU:HD11	1.80	0.64
20:A:1376:U:H2'	20:A:1377:A:C8	2.33	0.64
20:A:892:A:HO2'	20:A:1415:G:HO2'	1.37	0.64
23:Y:313:ALA:HA	23:Y:328:ILE:HA	1.80	0.64
9:J:56:HIS:O	9:J:58:ASP:N	2.30	0.63
1:B:52:GLU:OE1	1:B:56:ARG:NH2	2.31	0.63
23:Y:353:ALA:HB3	23:Y:378:VAL:HB	1.79	0.63
20:A:1271:G:H5'	20:A:1314:C:H5''	1.79	0.63
23:Y:163:VAL:HG22	23:Y:258:VAL:HB	1.81	0.63
23:Y:96:ARG:HA	23:Y:99:ARG:HB2	1.80	0.63
11:L:87:GLY:HA2	11:L:98:TYR:H	1.62	0.63
10:K:84:VAL:HG22	10:K:110:ASP:HA	1.79	0.63
23:Y:496:LYS:HA	23:Y:509:HIS:HA	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:93:ARG:HH21	20:A:1178:G:H5''	1.64	0.63
18:S:49:ILE:HD13	18:S:71:LEU:HD22	1.80	0.63
20:A:1481:U:H2'	20:A:1482:G:C8	2.33	0.63
6:G:78:ARG:HD2	6:G:79:ARG:HD3	1.80	0.63
10:K:113:PRO:HB3	20:A:676:A:H5''	1.80	0.63
8:I:113:LYS:HE2	20:A:1187:G:H5'	1.79	0.63
18:S:40:ILE:HG12	18:S:71:LEU:HD23	1.78	0.63
20:A:1324:A:H4'	20:A:1362:C:H4'	1.80	0.63
2:C:58:GLU:H	2:C:65:ALA:HB3	1.62	0.63
16:Q:61:GLU:HA	16:Q:71:PHE:HA	1.81	0.63
20:A:925:G:O2'	20:A:927:G:OP1	2.13	0.63
23:Y:259:PHE:HB2	23:Y:272:LEU:HD13	1.81	0.63
20:A:33:A:N1	20:A:551:U:O4	2.32	0.63
23:Y:31:ARG:NH2	23:Y:266:ASN:OD1	2.31	0.63
20:A:722:A:H4'	20:A:723:U:H5	1.62	0.63
10:K:116:HIS:CD2	20:A:674:G:H21	2.17	0.63
11:L:80:HIS:CE1	23:Y:425:SER:HB3	2.33	0.63
20:A:1522:U:H2'	20:A:1523:G:C8	2.34	0.63
1:B:174:VAL:O	1:B:177:ALA:N	2.32	0.63
8:I:93:ARG:NH2	20:A:1179:A:OP2	2.31	0.63
1:B:92:TYR:HE1	1:B:94:ASN:HB2	1.63	0.63
21:W:69:A:H2'	21:W:70:G:H8	1.63	0.63
3:D:62:GLN:O	3:D:65:ARG:N	2.31	0.63
20:A:312:C:H2'	20:A:313:A:C8	2.34	0.62
10:K:52:GLY:H	10:K:55:LYS:HE2	1.63	0.62
20:A:1083:U:H5''	20:A:1084:G:OP2	1.99	0.62
14:O:8:LYS:HE3	14:O:31:LEU:HD21	1.81	0.62
20:A:782:A:H62	20:A:800:G:H21	1.48	0.62
20:A:1435:G:H2'	20:A:1436:U:C6	2.34	0.62
8:I:20:ARG:O	8:I:60:ASP:N	2.22	0.62
4:E:93:PRO:HG3	7:H:105:ARG:HG2	1.80	0.62
20:A:406:G:H1	20:A:436:C:N4	1.93	0.62
20:A:890:G:H22	20:A:906:G:H2'	1.64	0.62
2:C:12:LEU:HD12	13:N:58:LYS:HB2	1.81	0.62
23:Y:134:ALA:HB3	23:Y:258:VAL:HA	1.82	0.62
20:A:1420:C:H42	20:A:1480:G:H1	1.48	0.62
4:E:32:VAL:HG13	4:E:62:ALA:HB2	1.79	0.62
4:E:151:LEU:HB3	7:H:79:VAL:HG22	1.80	0.62
20:A:1412:C:H2'	20:A:1413:A:C8	2.35	0.62
14:O:46:HIS:HB3	20:A:668:G:H1'	1.80	0.62
11:L:70:ILE:HG23	11:L:100:ILE:HD12	1.81	0.62
20:A:137:C:H42	20:A:226:G:H1	1.45	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:49:U:O4	20:A:362:G:N2	2.32	0.62
23:Y:83:ASP:C	23:Y:85:PRO:HD3	2.19	0.62
3:D:18:LYS:HB3	3:D:33:MET:HG3	1.81	0.62
1:B:69:LEU:H	1:B:163:PHE:H	1.47	0.62
3:D:81:GLU:HA	3:D:84:LYS:HE2	1.80	0.62
20:A:294:U:H2'	20:A:295:C:C6	2.34	0.62
20:A:666:G:OP2	20:A:725:G:N2	2.28	0.62
11:L:84:LEU:HD22	11:L:104:VAL:HG13	1.82	0.62
20:A:1270:C:H2'	20:A:1271:G:C8	2.35	0.62
21:W:6:C:H2'	21:W:7:G:C8	2.34	0.62
16:Q:57:VAL:HG12	16:Q:76:LEU:HA	1.81	0.62
11:L:93:LEU:HG	11:L:96:VAL:HG22	1.82	0.62
23:Y:330:VAL:HG13	23:Y:331:TYR:H	1.64	0.62
5:F:100:ASN:HA	17:R:23:LYS:HE3	1.82	0.62
1:B:152:PHE:HE2	1:B:155:LEU:HD12	1.65	0.62
23:Y:486:THR:OG1	23:Y:487:ILE:N	2.28	0.62
11:L:113:ARG:HH21	11:L:115:LYS:HB3	1.65	0.61
8:I:97:LYS:HD2	8:I:102:LEU:HD12	1.82	0.61
21:W:70:G:H2'	21:W:71:C:C6	2.35	0.61
20:A:1461:G:H2'	20:A:1462:G:H8	1.65	0.61
5:F:82:ARG:NH2	5:F:84:ASN:OD1	2.33	0.61
7:H:127:LEU:HB3	7:H:129:VAL:HG22	1.81	0.61
20:A:21:G:H2'	20:A:22:G:C8	2.34	0.61
4:E:33:VAL:HG12	4:E:112:LEU:HD12	1.82	0.61
4:E:143:ARG:NH1	7:H:77:GLU:OE1	2.33	0.61
1:B:166:ASP:HA	1:B:188:ALA:HB2	1.82	0.61
1:B:79:ASP:O	1:B:82:ARG:HG2	2.00	0.61
20:A:56:U:H2'	20:A:57:G:H8	1.65	0.61
19:T:43:LEU:HB2	19:T:52:ALA:HB2	1.81	0.61
13:N:48:ALA:HA	13:N:53:LEU:HB2	1.81	0.61
11:L:58:VAL:HG21	11:L:85:ILE:HD11	1.80	0.61
9:J:8:LEU:HA	9:J:96:ILE:HG22	1.80	0.61
17:R:48:GLY:O	17:R:74:ARG:NH2	2.32	0.61
12:M:78:ILE:HA	12:M:81:LEU:HB2	1.81	0.61
20:A:687:A:H62	20:A:703:G:N2	1.97	0.61
20:A:1201:A:H4'	20:A:1202:G:H5''	1.82	0.61
23:Y:680:PRO:O	23:Y:682:GLN:N	2.34	0.61
20:A:740:U:O2'	20:A:741:G:O4'	2.17	0.61
2:C:3:ASN:O	2:C:4:LYS:HB2	1.99	0.61
23:Y:161:PRO:HA	23:Y:256:THR:HB	1.81	0.61
3:D:64:LEU:HD13	3:D:198:VAL:HG11	1.83	0.61
20:A:1338:G:H21	21:W:41:A:H1'	1.65	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:707:C:H2'	20:A:708:C:H6	1.65	0.61
23:Y:605:ILE:HG13	23:Y:648:PRO:HA	1.83	0.61
23:Y:137:ASN:ND2	23:Y:263:ALA:H	1.89	0.61
20:A:520:A:H62	20:A:529:G:N2	1.98	0.61
20:A:339:C:H2'	20:A:340:U:C6	2.36	0.61
13:N:61:TRP:HZ2	20:A:1368:G:H4'	1.64	0.61
1:B:169:LYS:O	1:B:172:ILE:N	2.32	0.61
3:D:19:LEU:HD23	3:D:67:ILE:HB	1.82	0.61
20:A:1225:A:H2'	20:A:1226:C:C5	2.36	0.61
21:W:23:A:H2'	21:W:24:G:C8	2.36	0.61
5:F:46:ARG:HH22	17:R:37:VAL:HG21	1.66	0.61
14:O:67:LEU:HD13	14:O:87:ILE:HD12	1.83	0.61
3:D:25:ARG:NH2	20:A:411:A:OP2	2.33	0.60
1:B:223:ILE:O	1:B:227:GLY:N	2.34	0.60
20:A:1504:G:H4'	20:A:1505:G:H5'	1.83	0.60
20:A:810:C:H2'	20:A:811:C:C6	2.36	0.60
15:P:29:ASP:OD2	15:P:29:ASP:N	2.34	0.60
20:A:885:G:H1	20:A:912:C:H42	1.49	0.60
21:W:19:G:N2	21:W:56:C:N3	2.49	0.60
11:L:88:GLY:O	11:L:99:HIS:NE2	2.34	0.60
20:A:1198:G:H2'	20:A:1199:U:C6	2.36	0.60
23:Y:512:ILE:HA	23:Y:567:LEU:HA	1.82	0.60
2:C:163:ALA:HB3	20:A:1056:U:H4'	1.83	0.60
12:M:24:GLY:O	12:M:29:ARG:NH1	2.34	0.60
20:A:1081:G:H2'	20:A:1082:G:H8	1.66	0.60
20:A:865:A:H2'	20:A:866:C:C6	2.36	0.60
4:E:77:PRO:HD2	4:E:142:LEU:HD21	1.83	0.60
20:A:585:G:H1	20:A:756:C:N4	2.00	0.60
20:A:265:G:H2'	20:A:266:G:H5''	1.84	0.60
23:Y:135:PHE:HA	23:Y:260:LEU:HA	1.84	0.60
20:A:185:A:H2'	20:A:186:C:C6	2.36	0.60
23:Y:268:GLY:HA2	23:Y:271:LEU:HD21	1.83	0.60
23:Y:606:MET:HG3	23:Y:649:LEU:HD21	1.84	0.60
8:I:10:ARG:HD3	8:I:75:ASP:HB3	1.83	0.60
1:B:71:VAL:HB	1:B:164:VAL:HG22	1.84	0.60
11:L:54:LYS:HD2	11:L:70:ILE:HG12	1.83	0.60
21:W:41:A:H2'	21:W:42:U:C6	2.37	0.60
20:A:1238:A:H2	20:A:1241:G:N3	1.99	0.60
20:A:576:G:N7	20:A:881:G:H1'	2.16	0.60
20:A:1270:C:H2'	20:A:1271:G:H8	1.66	0.60
2:C:22:TRP:HB3	2:C:59:ARG:H	1.67	0.60
20:A:1288:A:H2'	20:A:1289:A:O4'	2.02	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:31:CYS:HB3	3:D:33:MET:HG2	1.83	0.60
20:A:588:G:H1	20:A:651:C:H42	1.50	0.60
20:A:33:A:H4'	20:A:364:A:H1'	1.83	0.59
9:J:42:THR:H	20:A:1151:A:H5''	1.66	0.59
10:K:41:THR:HG21	10:K:71:LYS:HD3	1.83	0.59
20:A:1290:G:H3'	20:A:1291:G:H8	1.66	0.59
20:A:1206:G:H2'	20:A:1207:G:O4'	2.02	0.59
7:H:103:VAL:HG12	7:H:138:TRP:HD1	1.67	0.59
11:L:58:VAL:HG12	11:L:60:LEU:N	2.10	0.59
5:F:82:ARG:HB2	5:F:85:VAL:HG23	1.83	0.59
7:H:111:ILE:HD11	7:H:137:VAL:HG23	1.83	0.59
20:A:217:C:H2'	20:A:218:C:H6	1.67	0.59
16:Q:66:SER:OG	20:A:254:G:OP1	2.20	0.59
20:A:1230:C:H2'	20:A:1231:G:H8	1.68	0.59
20:A:1266:G:N2	20:A:1269:A:OP2	2.34	0.59
17:R:75:ILE:HD11	20:A:735:C:H1'	1.84	0.59
20:A:505:G:H1	20:A:526:C:N4	2.00	0.59
4:E:17:ALA:HA	4:E:26:PHE:HA	1.83	0.59
20:A:801:U:H2'	20:A:802:A:C8	2.37	0.59
20:A:898:G:N2	20:A:901:A:OP2	2.36	0.59
2:C:25:GLY:O	2:C:27:LYS:N	2.35	0.59
20:A:919:A:O2'	20:A:1080:A:N1	2.31	0.59
11:L:93:LEU:HD21	11:L:96:VAL:HG13	1.84	0.59
20:A:129(A):G:H4'	20:A:130:A:H5''	1.84	0.59
20:A:308:C:H2'	20:A:309:G:H8	1.67	0.59
20:A:861:G:HO2'	20:A:874:G:HO2'	1.50	0.59
14:O:82:ILE:HG12	14:O:87:ILE:H	1.67	0.59
1:B:61:LEU:O	1:B:65:GLY:N	2.32	0.59
11:L:49:ASN:HD21	20:A:528:C:N4	2.01	0.59
3:D:172:PRO:HB2	3:D:187:ARG:HH22	1.68	0.59
16:Q:3:LYS:NZ	20:A:128:G:O2'	2.35	0.59
20:A:1103:C:H2'	20:A:1104:G:O4'	2.03	0.59
8:I:16:ARG:NH1	20:A:1147:C:O2	2.35	0.59
11:L:34:ARG:HB2	20:A:363:A:OP1	2.03	0.59
20:A:241:C:H2'	20:A:242:C:C6	2.38	0.59
15:P:20:VAL:HG23	15:P:35:LYS:HA	1.85	0.59
14:O:7:GLU:O	14:O:10:LYS:HG3	2.03	0.59
23:Y:309:LEU:HA	23:Y:333:GLY:HA3	1.83	0.59
20:A:576:G:OP2	20:A:577:G:H5''	2.03	0.59
20:A:131:C:H2'	20:A:132:C:C6	2.38	0.59
18:S:12:ASP:OD1	18:S:14:HIS:NE2	2.35	0.59
1:B:42:ILE:HD11	1:B:202:PRO:HB2	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:T:66:ALA:HB1	19:T:72:LEU:HB2	1.84	0.59
23:Y:216:LEU:HD11	23:Y:246:ILE:HD11	1.83	0.59
10:K:85:ARG:HA	10:K:110:ASP:O	2.03	0.58
25:Y:701:FUA:H201	25:Y:701:FUA:O1	2.03	0.58
15:P:80:PHE:HB3	20:A:458(E):A:H5''	1.85	0.58
20:A:950:U:H2'	20:A:951:G:C8	2.38	0.58
5:F:11:ASN:HB3	5:F:14:LEU:HG	1.84	0.58
7:H:14:ARG:HD3	7:H:82:HIS:HE1	1.68	0.58
10:K:123:LYS:HA	10:K:126:ARG:HB3	1.85	0.58
20:A:946:A:H2'	20:A:947:G:H8	1.67	0.58
20:A:216:G:H2'	20:A:217:C:C6	2.38	0.58
20:A:272:C:H2'	20:A:273:A:C8	2.38	0.58
20:A:1114:C:H2'	20:A:1115:C:H6	1.69	0.58
20:A:1306:A:N6	20:A:1331:G:O2'	2.35	0.58
23:Y:368:GLU:O	23:Y:370:LYS:NZ	2.33	0.58
3:D:157:LEU:O	3:D:161:ASN:ND2	2.34	0.58
23:Y:524:GLU:HB2	23:Y:564:LYS:HA	1.86	0.58
10:K:20:TYR:HB2	10:K:31:THR:HG23	1.86	0.58
12:M:34:LEU:HD13	12:M:41:PRO:HG3	1.86	0.58
20:A:1513:A:H2'	20:A:1514:C:C6	2.39	0.58
1:B:75:LYS:O	1:B:78:GLN:HB3	2.04	0.58
12:M:86:CYS:O	12:M:90:LEU:N	2.34	0.58
23:Y:69:VAL:HA	23:Y:81:ILE:O	2.03	0.58
11:L:45:PRO:HG3	11:L:92:ASP:HB3	1.86	0.58
20:A:356:A:N3	20:A:368:U:O2'	2.29	0.58
8:I:11:LYS:HG3	8:I:108:VAL:HA	1.86	0.58
12:M:97:PRO:HA	12:M:110:ARG:HG3	1.86	0.58
3:D:10:ARG:NH2	20:A:543:C:OP2	2.28	0.58
6:G:54:THR:OG1	6:G:55:GLY:N	2.36	0.58
7:H:119:LEU:HB2	7:H:124:ALA:HB2	1.85	0.58
20:A:410:G:N1	20:A:431:A:OP2	2.31	0.58
23:Y:565:VAL:HG12	23:Y:566:THR:O	2.03	0.58
20:A:689:C:H2'	20:A:690:G:O4'	2.04	0.58
20:A:815:A:N6	20:A:1508:G:H21	2.01	0.58
20:A:1510:U:H2'	20:A:1511:G:C8	2.39	0.58
1:B:162:ILE:HD11	1:B:184:VAL:HG13	1.85	0.58
20:A:1002:G:H2'	20:A:1003:G:C8	2.38	0.58
23:Y:114:VAL:HB	23:Y:116:PRO:HD3	1.86	0.58
1:B:15:VAL:HB	1:B:209:ARG:HE	1.68	0.58
20:A:1488:G:H2'	20:A:1489:G:H8	1.69	0.57
3:D:101:LEU:HD22	3:D:138:TYR:HD2	1.69	0.57
20:A:1422:G:H2'	20:A:1423:G:H8	1.69	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:Q:59:ILE:HG12	16:Q:73:VAL:HG22	1.86	0.57
20:A:1062:U:H2'	20:A:1063:C:C6	2.39	0.57
20:A:406:G:H2'	20:A:407:G:H8	1.69	0.57
23:Y:512:ILE:HG22	23:Y:567:LEU:HD13	1.86	0.57
20:A:234:C:H2'	20:A:235:C:C6	2.40	0.57
6:G:15:ASP:HB3	6:G:19:GLY:H	1.69	0.57
4:E:50:GLU:HG2	4:E:52:PRO:HD2	1.85	0.57
20:A:280:C:H3'	20:A:281:G:H5'	1.85	0.57
16:Q:70:ARG:HG2	20:A:235:C:H5'	1.86	0.57
4:E:19:MET:SD	20:A:15:G:H1'	2.43	0.57
4:E:20:GLN:H	4:E:24:ARG:HA	1.68	0.57
20:A:1218:C:H2'	20:A:1219:U:C6	2.40	0.57
20:A:1480:G:C2	20:A:1481:U:H1'	2.39	0.57
20:A:890:G:N2	20:A:906:G:H2'	2.19	0.57
4:E:27:ARG:HE	4:E:49:PRO:HD3	1.69	0.57
20:A:935:A:H2'	20:A:936:C:H6	1.68	0.57
1:B:71:VAL:HA	1:B:93:VAL:HB	1.86	0.57
20:A:757:U:H2'	20:A:758:G:O4'	2.05	0.57
19:T:51:GLU:HA	19:T:54:LYS:HD2	1.85	0.57
20:A:302:G:N3	20:A:556:C:H4'	2.20	0.57
23:Y:259:PHE:CE1	23:Y:275:ALA:HB1	2.40	0.57
20:A:1287:A:H2'	20:A:1288:A:C8	2.40	0.57
7:H:100:ILE:HG22	7:H:125:ARG:HH21	1.68	0.57
20:A:68(G):G:C4	20:A:68(H):G:H1'	2.40	0.57
20:A:992:U:H3	20:A:1044:A:H62	1.50	0.57
20:A:68(P):C:H2'	20:A:68(Q):U:O4'	2.05	0.57
20:A:1118:C:H2'	20:A:1119:C:H6	1.69	0.57
20:A:1401:G:H2'	20:A:1402:C:O4'	2.04	0.57
3:D:23:GLY:O	3:D:25:ARG:N	2.36	0.57
21:W:17:U:H5'	21:W:18:G:C4'	2.34	0.57
20:A:813:U:H2'	20:A:814:A:C8	2.39	0.57
20:A:891:U:H2'	20:A:892:A:C8	2.40	0.57
15:P:81:ARG:HG2	15:P:83:GLU:H	1.69	0.57
20:A:707:C:H2'	20:A:708:C:C6	2.39	0.57
1:B:157:ARG:HH11	1:B:157:ARG:HB3	1.69	0.57
21:W:63:C:H2'	21:W:64:G:H8	1.70	0.57
10:K:111:ASP:O	10:K:113:PRO:HD3	2.05	0.57
2:C:7:PRO:HG2	2:C:201:TYR:CE2	2.39	0.57
20:A:1286:A:N6	20:A:1355:G:OP1	2.37	0.57
23:Y:107:VAL:HG22	23:Y:135:PHE:HB3	1.87	0.57
23:Y:136:ALA:HB3	23:Y:260:LEU:HB2	1.86	0.57
17:R:58:LEU:HD22	17:R:58:LEU:H	1.69	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:813:U:H2'	20:A:814:A:H8	1.69	0.57
11:L:17:LYS:NZ	20:A:302:G:O3'	2.33	0.57
23:Y:272:LEU:HA	23:Y:275:ALA:HB3	1.87	0.57
1:B:87:ARG:HG2	1:B:223:ILE:HD11	1.86	0.57
20:A:552:U:H2'	20:A:553:A:H8	1.68	0.57
2:C:106:VAL:HG12	2:C:108:ASN:H	1.68	0.57
20:A:745:C:H2'	20:A:746:A:H8	1.69	0.57
9:J:49:VAL:HG23	13:N:41:ARG:HB2	1.87	0.57
9:J:39:PRO:HA	9:J:70:ARG:HG3	1.87	0.57
12:M:122:LYS:HA	20:A:954:G:H5'	1.86	0.57
20:A:1522:U:H2'	20:A:1523:G:H8	1.69	0.57
8:I:107:ARG:HE	20:A:1347:G:H5''	1.70	0.57
20:A:1510:U:H2'	20:A:1511:G:H8	1.70	0.56
23:Y:8:ASP:O	23:Y:9:LEU:HB2	2.04	0.56
9:J:51:ARG:HG2	9:J:59:SER:O	2.05	0.56
23:Y:564:LYS:HG2	23:Y:565:VAL:H	1.69	0.56
2:C:7:PRO:O	2:C:11:ARG:HG2	2.04	0.56
21:W:41:A:O2'	21:W:42:U:OP1	2.21	0.56
20:A:321:A:H61	20:A:332:G:H1	1.53	0.56
20:A:1262:C:H2'	20:A:1263:C:C6	2.39	0.56
16:Q:95:TYR:OH	20:A:279:A:OP2	2.15	0.56
20:A:1507:A:H2'	20:A:1508:G:C8	2.40	0.56
11:L:36:VAL:N	11:L:58:VAL:HA	2.19	0.56
11:L:52:LEU:HG	11:L:53:ARG:H	1.70	0.56
12:M:87:TYR:HE1	18:S:76:PRO:HA	1.70	0.56
23:Y:610:VAL:O	23:Y:642:VAL:HA	2.05	0.56
17:R:70:ILE:O	17:R:74:ARG:HG3	2.04	0.56
20:A:1040:U:H2'	20:A:1041:A:H8	1.69	0.56
20:A:318:G:H2'	20:A:319:G:H8	1.69	0.56
23:Y:149:VAL:O	23:Y:153:MET:HG3	2.05	0.56
12:M:2:ALA:O	12:M:4:ILE:N	2.37	0.56
23:Y:25:LYS:HE3	26:Y:702:GDP:O2B	2.05	0.56
14:O:42:HIS:NE2	20:A:739:C:O2	2.38	0.56
20:A:309:G:H2'	20:A:310:G:H8	1.70	0.56
20:A:1363:A:H4'	20:A:1364:U:H5''	1.86	0.56
5:F:33:TYR:HA	5:F:71:ARG:HH21	1.69	0.56
23:Y:534:ILE:HG23	23:Y:538:TYR:HD2	1.70	0.56
23:Y:544:LYS:O	23:Y:548:GLU:N	2.36	0.56
20:A:520:A:N6	20:A:529:G:H21	2.04	0.56
20:A:924:C:H2'	20:A:925:G:C8	2.40	0.56
19:T:89:ARG:NH1	19:T:105:SER:O	2.38	0.56
7:H:97:VAL:HG13	7:H:98:LYS:H	1.71	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1124:G:O2'	20:A:1145:C:N4	2.39	0.56
20:A:1144:G:N2	20:A:1146:A:H62	2.03	0.56
20:A:828:A:H2'	20:A:829:G:O4'	2.05	0.56
20:A:318:G:H2'	20:A:319:G:C8	2.41	0.56
18:S:13:ASP:O	18:S:17:GLU:HG2	2.04	0.56
21:W:64:G:C6	21:W:65:U:O4	2.59	0.56
11:L:5:PRO:HG2	11:L:15:ARG:HH21	1.69	0.56
11:L:114:LYS:HB2	20:A:538:G:H5''	1.86	0.56
20:A:591:U:H2'	20:A:592:G:C8	2.41	0.56
2:C:153:VAL:HG12	2:C:198:VAL:HG22	1.88	0.56
14:O:65:ARG:NH2	20:A:581:G:OP1	2.38	0.56
20:A:408:A:H2	20:A:434:U:H3	1.53	0.56
21:W:63:C:H2'	21:W:64:G:C8	2.41	0.56
23:Y:207:ASP:HA	23:Y:210:ARG:HB2	1.87	0.56
20:A:584:G:H2'	20:A:585:G:C8	2.41	0.56
4:E:24:ARG:HD2	22:V:26:A:H2	1.70	0.56
7:H:120:THR:HG23	7:H:123:GLU:HG3	1.86	0.56
20:A:217:C:H2'	20:A:218:C:C6	2.41	0.56
20:A:565:U:OP2	20:A:566:G:O2'	2.24	0.56
19:T:21:LYS:O	19:T:24:LEU:HB3	2.06	0.56
20:A:1026:G:O6	20:A:1035:A:N1	2.39	0.56
11:L:37:CYS:HA	11:L:57:LYS:H	1.71	0.55
23:Y:512:ILE:HD12	23:Y:589:ALA:HB1	1.87	0.55
21:W:68:U:H2'	21:W:69:A:C8	2.41	0.55
20:A:950:U:H2'	20:A:951:G:H8	1.71	0.55
23:Y:20:HIS:HB3	23:Y:118:SER:N	2.21	0.55
23:Y:178:ILE:HA	23:Y:185:ALA:HA	1.88	0.55
23:Y:466:LEU:O	23:Y:471:LYS:N	2.40	0.55
3:D:136:PRO:HD2	20:A:403:C:H5''	1.88	0.55
23:Y:146:LEU:O	23:Y:150:ILE:HG12	2.06	0.55
2:C:78:GLY:HA3	2:C:83:ARG:H	1.71	0.55
20:A:980:C:H5'	20:A:981:U:C5	2.41	0.55
1:B:71:VAL:H	1:B:164:VAL:HA	1.72	0.55
23:Y:526:VAL:O	23:Y:528:ALA:N	2.40	0.55
20:A:1488:G:H2'	20:A:1489:G:C8	2.41	0.55
18:S:36:ARG:HH22	18:S:75:ALA:HB3	1.71	0.55
2:C:191:THR:HG23	2:C:196:LEU:HD21	1.88	0.55
3:D:196:LEU:O	3:D:198:VAL:N	2.40	0.55
11:L:86:ARG:HE	11:L:99:HIS:HB2	1.72	0.55
8:I:11:LYS:HA	8:I:108:VAL:HG12	1.87	0.55
7:H:9:MET:HG3	7:H:26:VAL:HG11	1.88	0.55
20:A:1145:C:O2'	20:A:1146:A:O5'	2.24	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:110:LEU:O	4:E:115:VAL:HG23	2.06	0.55
11:L:71:PRO:HD2	11:L:102:ARG:HD3	1.89	0.55
7:H:89:PRO:HG2	20:A:878:G:H5'	1.87	0.55
20:A:802:A:H2'	20:A:803:G:O4'	2.07	0.55
20:A:1304:G:N1	20:A:1332:A:OP2	2.40	0.55
18:S:76:PRO:O	18:S:78:ARG:N	2.37	0.55
23:Y:70:THR:HB	23:Y:81:ILE:HD13	1.88	0.55
16:Q:45:HIS:CB	16:Q:72:ARG:HA	2.36	0.55
18:S:54:GLY:HA3	20:A:1220:G:H21	1.72	0.55
20:A:503:C:H2'	20:A:504:C:C6	2.42	0.55
12:M:14:ARG:NH1	20:A:1295:G:O2'	2.39	0.55
20:A:1172:C:H2'	20:A:1173:G:C8	2.41	0.55
5:F:47:ARG:HA	5:F:57:GLN:HA	1.87	0.55
4:E:91:LEU:HD22	4:E:120:THR:HB	1.89	0.55
20:A:454:C:N4	20:A:479:C:N3	2.55	0.55
16:Q:29:HIS:CG	16:Q:32:TYR:HB2	2.42	0.55
20:A:160:A:H61	20:A:347:G:H1'	1.72	0.55
3:D:33:MET:O	3:D:35:ARG:N	2.40	0.55
1:B:91:PRO:HG2	1:B:155:LEU:HD23	1.89	0.55
20:A:891:U:H2'	20:A:892:A:H8	1.71	0.55
20:A:185:A:H2'	20:A:186:C:H6	1.72	0.55
16:Q:56:VAL:HB	16:Q:78:GLU:HG2	1.88	0.55
20:A:109:A:H62	20:A:324:G:H21	1.55	0.55
20:A:715:A:H2'	20:A:716:A:C8	2.41	0.55
23:Y:25:LYS:HE3	26:Y:702:GDP:PB	2.47	0.55
20:A:578:C:H2'	20:A:579:G:C8	2.42	0.55
1:B:24:TRP:CZ3	1:B:26:PRO:HA	2.41	0.55
12:M:3:ARG:HH21	12:M:7:VAL:HG22	1.71	0.55
23:Y:110:SER:HB3	23:Y:144:ALA:HA	1.89	0.55
20:A:242:C:H2'	20:A:245:C:H5	1.72	0.55
2:C:155:GLY:HA3	2:C:196:LEU:HA	1.89	0.55
8:I:124:GLN:HB3	20:A:1232:U:H5"	1.88	0.55
7:H:110:ALA:HB3	7:H:121:ASP:HB3	1.89	0.55
10:K:72:ALA:HB1	10:K:77:MET:HG2	1.90	0.54
20:A:1324:A:H2'	20:A:1325:C:C6	2.41	0.54
20:A:1436:U:H2'	20:A:1437:C:O4'	2.07	0.54
14:O:11:VAL:HG21	14:O:34:LEU:HD22	1.88	0.54
23:Y:291:GLY:HA2	23:Y:400:GLU:N	2.22	0.54
18:S:64:GLU:O	18:S:67:VAL:HG23	2.06	0.54
7:H:37:ARG:O	7:H:41:ARG:HB2	2.07	0.54
7:H:46:LYS:HB3	7:H:62:TYR:HB2	1.89	0.54
10:K:82:VAL:HG21	10:K:105:VAL:HG12	1.88	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:P:53:VAL:HG12	15:P:79:VAL:HG22	1.88	0.54
20:A:476:G:H2'	20:A:477:G:C8	2.43	0.54
1:B:162:ILE:HG12	1:B:184:VAL:HA	1.88	0.54
20:A:299:G:C6	20:A:300:A:C6	2.95	0.54
23:Y:487:ILE:HB	23:Y:597:GLY:O	2.08	0.54
10:K:79:SER:HA	10:K:104:GLN:HB3	1.89	0.54
23:Y:294:PRO:HD3	23:Y:397:VAL:HG12	1.90	0.54
20:A:115:G:O2'	20:A:116:A:OP2	2.25	0.54
11:L:76:ASN:O	11:L:78:GLN:N	2.31	0.54
20:A:22:G:H2'	20:A:23:C:C6	2.43	0.54
20:A:1040:U:H2'	20:A:1041:A:C8	2.42	0.54
16:Q:56:VAL:HG23	16:Q:81:ARG:HG3	1.88	0.54
7:H:31:PHE:HE1	20:A:642:A:HO2'	1.55	0.54
3:D:25:ARG:HB2	20:A:410:G:OP2	2.07	0.54
1:B:184:VAL:N	1:B:198:ASP:HB2	2.22	0.54
17:R:49:LYS:HB3	20:A:719:C:O2'	2.08	0.54
12:M:74:VAL:O	12:M:78:ILE:HG12	2.07	0.54
19:T:22:ARG:NE	20:A:324:G:OP1	2.38	0.54
10:K:118:GLY:HA2	20:A:716:A:H1'	1.88	0.54
20:A:1048:G:H2'	20:A:1050:G:H8	1.71	0.54
23:Y:13:ARG:O	23:Y:80:ASN:N	2.31	0.54
20:A:1440(J):C:H1'	20:A:1440(K):G:N2	2.22	0.54
23:Y:18:ALA:HB2	23:Y:85:PRO:HD2	1.89	0.54
21:W:17:U:H5'	21:W:18:G:O4'	2.07	0.54
11:L:69:TYR:CD1	11:L:70:ILE:HG13	2.43	0.54
23:Y:289:ILE:HB	23:Y:301:ILE:HB	1.90	0.54
20:A:216:G:H2'	20:A:217:C:H6	1.73	0.54
20:A:1511:G:H2'	20:A:1512:U:O4'	2.08	0.54
1:B:70:PHE:CD2	1:B:81:VAL:HB	2.43	0.54
11:L:52:LEU:HG	11:L:54:LYS:HZ1	1.72	0.54
3:D:15:GLU:HG3	3:D:66:ARG:HH22	1.72	0.54
5:F:95:GLU:O	5:F:97:PHE:N	2.41	0.54
1:B:69:LEU:CB	1:B:162:ILE:HG22	2.35	0.54
3:D:11:LEU:HD13	3:D:66:ARG:HD2	1.90	0.54
20:A:1084:G:H3'	20:A:1085:U:H2'	1.90	0.54
7:H:14:ARG:HE	7:H:83:ILE:HG23	1.73	0.54
20:A:678:U:H1'	20:A:777:A:O3'	2.08	0.54
19:T:78:ALA:HA	19:T:81:LYS:HD3	1.88	0.54
20:A:352:C:O2	20:A:355:C:N4	2.41	0.54
20:A:1097:C:H2'	20:A:1098:C:C6	2.43	0.54
20:A:687:A:N6	20:A:703:G:H21	2.01	0.54
8:I:99:LEU:HD12	8:I:101:PHE:HE1	1.74	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:32:VAL:HG11	4:E:58:ALA:C	2.28	0.54
23:Y:467:LYS:HA	23:Y:471:LYS:HA	1.88	0.54
20:A:160:A:N6	20:A:347:G:H1'	2.23	0.54
7:H:91:ARG:O	7:H:93:VAL:N	2.40	0.54
8:I:112:LYS:NZ	8:I:116:LYS:O	2.32	0.54
4:E:146:ALA:O	4:E:150:ARG:HG2	2.08	0.54
1:B:167:PRO:HD2	1:B:188:ALA:CB	2.38	0.53
20:A:1440(J):C:O2'	20:A:1440(K):G:H5''	2.09	0.53
7:H:94:TYR:OH	20:A:597:G:N2	2.34	0.53
17:R:45:SER:OG	17:R:46:GLU:N	2.42	0.53
20:A:119:A:H4'	20:A:120:A:C8	2.42	0.53
20:A:68(Y):C:H2'	20:A:101:A:C8	2.43	0.53
23:Y:262:SER:N	23:Y:267:LYS:O	2.41	0.53
11:L:53:ARG:HG3	11:L:69:TYR:CE1	2.43	0.53
20:A:974:A:H8	20:A:974:A:OP1	1.91	0.53
20:A:115:G:H1'	20:A:116:A:N7	2.22	0.53
20:A:1097:C:H2'	20:A:1098:C:H6	1.71	0.53
3:D:51:PRO:HB2	3:D:56:VAL:HG13	1.90	0.53
2:C:86:VAL:O	2:C:90:GLU:HG3	2.08	0.53
20:A:1176:A:H2'	20:A:1177:G:C8	2.44	0.53
20:A:730:G:H5'	20:A:816:A:O2'	2.08	0.53
8:I:14:VAL:HG11	20:A:1148:U:H4'	1.89	0.53
20:A:552:U:H2'	20:A:553:A:C8	2.44	0.53
11:L:82:VAL:HB	11:L:105:TYR:HB2	1.89	0.53
20:A:243:A:H4'	20:A:244:U:O5'	2.07	0.53
12:M:87:TYR:CE1	18:S:76:PRO:HA	2.44	0.53
7:H:94:TYR:CG	20:A:598:U:H4'	2.42	0.53
20:A:777:A:H2'	20:A:778:G:H8	1.72	0.53
20:A:415:A:H2'	20:A:416:G:H8	1.72	0.53
23:Y:201:ILE:HD13	23:Y:206:LEU:HD12	1.91	0.53
20:A:1003:G:O6	20:A:1037:C:N3	2.41	0.53
11:L:15:ARG:HB3	20:A:562:C:H1'	1.90	0.53
1:B:131:PRO:HB2	1:B:134:GLU:HB2	1.91	0.53
15:P:21:VAL:HG11	15:P:59:TRP:NE1	2.24	0.53
23:Y:247:ARG:HB2	23:Y:279:TYR:HD1	1.73	0.53
12:M:80:ARG:HA	12:M:83:ASP:HB3	1.90	0.53
12:M:80:ARG:HB3	18:S:65:ASN:HB3	1.90	0.53
20:A:748:C:O2'	20:A:749:C:OP2	2.18	0.53
20:A:108:G:OP1	20:A:326:G:N2	2.40	0.53
3:D:193:ASP:OD1	3:D:193:ASP:N	2.40	0.53
20:A:68(H):G:H1	20:A:68(R):C:H42	1.56	0.53
20:A:328:C:H4'	20:A:329:A:H5'	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:M:14:ARG:NH1	20:A:1302:U:O4	2.41	0.53
20:A:149:A:H2'	20:A:150:C:C6	2.44	0.53
23:Y:443:HIS:HB2	23:Y:450:ILE:HD11	1.91	0.53
20:A:830:G:H2'	20:A:831:U:O4'	2.08	0.53
23:Y:22:ASP:O	26:Y:702:GDP:PB	2.67	0.53
4:E:131:ILE:O	4:E:135:THR:OG1	2.21	0.53
3:D:72:GLU:OE2	3:D:207:TYR:OH	2.25	0.53
20:A:46:G:O2'	20:A:365:U:O2'	2.14	0.53
20:A:777:A:H2'	20:A:778:G:C8	2.44	0.53
23:Y:274:ASP:HA	23:Y:277:VAL:HG12	1.91	0.53
20:A:1018:C:H2'	20:A:1019:C:C6	2.44	0.53
7:H:52:ASP:OD2	7:H:56:LYS:N	2.42	0.53
1:B:167:PRO:HD2	1:B:188:ALA:HB3	1.91	0.53
1:B:176:GLU:O	1:B:180:LEU:HD12	2.08	0.53
17:R:74:ARG:HG2	17:R:79:LEU:HB3	1.91	0.53
9:J:91:PRO:O	9:J:93:GLY:N	2.42	0.53
7:H:128:GLY:O	20:A:600:C:H4'	2.09	0.53
20:A:1020:U:H2'	20:A:1021:G:H8	1.73	0.53
8:I:71:SER:HB3	20:A:1372:U:H5''	1.91	0.53
1:B:115:LEU:HB2	1:B:145:LEU:HG	1.90	0.53
20:A:1095:U:H2'	20:A:1096:C:C6	2.43	0.53
2:C:13:GLY:HA2	13:N:57:ARG:HH21	1.74	0.53
23:Y:25:LYS:N	26:Y:702:GDP:O2B	2.41	0.53
1:B:168:THR:C	1:B:171:ALA:H	2.12	0.53
11:L:92:ASP:OD2	20:A:523:A:N6	2.30	0.53
10:K:40:ILE:HA	20:A:685:G:H4'	1.91	0.53
4:E:19:MET:SD	4:E:24:ARG:HB3	2.48	0.53
20:A:1332:A:H2'	20:A:1333:A:O4'	2.08	0.53
23:Y:93:GLU:O	23:Y:97:SER:OG	2.27	0.53
20:A:401:C:H2'	20:A:402:G:C8	2.44	0.53
15:P:43:LYS:NZ	20:A:452:A:OP1	2.42	0.53
5:F:2:ARG:NH1	5:F:69:GLU:OE1	2.41	0.53
4:E:10:MET:N	4:E:10:MET:SD	2.77	0.53
3:D:25:ARG:N	20:A:409:G:OP1	2.40	0.53
20:A:1064:G:N2	20:A:1190:G:O2'	2.41	0.53
20:A:264:U:H2'	20:A:265:G:O4'	2.09	0.53
16:Q:67:LYS:O	16:Q:68:ARG:HB3	2.09	0.53
5:F:46:ARG:HB3	5:F:60:PHE:HE1	1.73	0.53
20:A:1118:C:H2'	20:A:1119:C:C6	2.44	0.53
23:Y:20:HIS:HB2	23:Y:117:GLN:HB3	1.91	0.53
20:A:1404:C:H1'	20:A:1499:A:C2	2.43	0.53
2:C:39:ILE:O	2:C:43:LEU:HG	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:151:A:N7	20:A:170:U:O4	2.42	0.53
20:A:1070:U:H2'	20:A:1071:C:C6	2.44	0.53
20:A:937:A:H2	20:A:1377:A:HO2'	1.57	0.53
23:Y:266:ASN:OD1	23:Y:266:ASN:N	2.39	0.53
23:Y:421:GLN:O	23:Y:424:LEU:HG	2.09	0.53
20:A:1340:A:C2	20:A:1341:U:C2	2.97	0.53
23:Y:180:VAL:HG12	23:Y:209:ALA:HB1	1.91	0.53
20:A:1533:C:H5	22:V:12:A:H61	1.55	0.53
10:K:84:VAL:N	10:K:109:VAL:O	2.42	0.52
23:Y:317:MET:HB2	23:Y:327:PHE:CE2	2.44	0.52
1:B:96:ARG:HG2	20:A:1099:G:OP1	2.09	0.52
20:A:1063:C:H42	20:A:1193:G:H1	1.57	0.52
6:G:24:THR:HA	6:G:27:ILE:HB	1.90	0.52
20:A:983:A:H2	20:A:984:C:C5	2.25	0.52
8:I:121:ARG:NH1	20:A:1343:G:O2'	2.43	0.52
9:J:82:ILE:O	9:J:86:MET:HB2	2.09	0.52
19:T:79:ARG:O	19:T:82:SER:OG	2.25	0.52
11:L:60:LEU:HD23	11:L:63:GLY:O	2.09	0.52
20:A:908:A:H2'	20:A:909:A:H8	1.73	0.52
20:A:673:G:H2'	20:A:674:G:H8	1.73	0.52
20:A:32:A:H2'	20:A:33:A:C8	2.44	0.52
20:A:1137:C:H4'	20:A:1138:G:C2	2.44	0.52
15:P:70:ALA:O	15:P:74:LEU:HG	2.09	0.52
20:A:572:A:HO2'	20:A:916:G:HO2'	1.52	0.52
2:C:160:ALA:O	2:C:162:GLN:N	2.42	0.52
6:G:3:ARG:NH1	20:A:1380:U:O2'	2.42	0.52
2:C:37:GLN:NE2	2:C:37:GLN:O	2.42	0.52
14:O:5:LYS:O	14:O:9:GLN:HG2	2.09	0.52
1:B:71:VAL:O	1:B:165:VAL:HG23	2.09	0.52
9:J:55:LYS:HG3	20:A:973:G:O4'	2.09	0.52
23:Y:13:ARG:HB2	23:Y:79:ILE:HG12	1.91	0.52
23:Y:309:LEU:HD21	23:Y:335:LEU:HD13	1.89	0.52
3:D:10:ARG:HA	3:D:13:ARG:HD2	1.91	0.52
6:G:27:ILE:HG21	6:G:36:LYS:HZ3	1.74	0.52
15:P:6:LEU:HB3	15:P:17:TYR:HD2	1.75	0.52
12:M:52:GLU:HA	12:M:55:ARG:HE	1.73	0.52
1:B:106:LYS:HD2	1:B:106:LYS:H	1.75	0.52
2:C:56:ASP:OD1	2:C:56:ASP:N	2.42	0.52
20:A:815:A:H61	20:A:1508:G:H21	1.57	0.52
3:D:126:ILE:HG23	3:D:146:ILE:HG23	1.92	0.52
20:A:1127:G:H1'	20:A:1148:U:C4	2.44	0.52
20:A:1137:C:H5'	20:A:1138:G:C6	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:827:U:O2'	20:A:859:A:N1	2.36	0.52
8:I:6:GLY:HA3	8:I:80:GLY:O	2.10	0.52
3:D:145:GLU:OE1	3:D:182:LYS:HB3	2.09	0.52
4:E:83:GLU:HG3	4:E:87:SER:O	2.09	0.52
3:D:61:LYS:HG2	3:D:75:PHE:HE2	1.73	0.52
16:Q:45:HIS:H	16:Q:72:ARG:HA	1.75	0.52
20:A:924:C:H2'	20:A:925:G:H8	1.75	0.52
7:H:31:PHE:HZ	7:H:113:SER:HB2	1.74	0.52
23:Y:175:SER:O	23:Y:187:THR:OG1	2.25	0.52
23:Y:481:VAL:HB	23:Y:483:TYR:CZ	2.44	0.52
23:Y:98:MET:HG3	23:Y:101:LEU:HD12	1.90	0.52
20:A:767:A:O2'	20:A:1524:C:O2	2.21	0.52
14:O:39:LEU:HD22	14:O:42:HIS:HB3	1.90	0.52
20:A:559:A:H4'	20:A:560:U:H3'	1.91	0.52
23:Y:311:ALA:HA	23:Y:330:VAL:HA	1.91	0.52
23:Y:243:VAL:HA	23:Y:279:TYR:HE1	1.73	0.52
20:A:572:A:O2'	20:A:916:G:O2'	2.26	0.52
23:Y:66:THR:O	23:Y:363:ARG:NH2	2.42	0.52
20:A:20:U:O2'	20:A:573:A:N6	2.42	0.52
20:A:1507:A:H2'	20:A:1508:G:H8	1.75	0.52
11:L:83:VAL:HB	11:L:100:ILE:HG23	1.92	0.52
23:Y:607:ARG:HG2	23:Y:646:PHE:HE1	1.74	0.52
23:Y:100:VAL:HG21	23:Y:314:PHE:CZ	2.44	0.52
20:A:1349:A:H2'	20:A:1350:A:O4'	2.09	0.52
23:Y:611:THR:HA	23:Y:642:VAL:HG22	1.90	0.52
17:R:58:LEU:HB3	17:R:62:GLU:HB3	1.92	0.52
6:G:31:MET:HG3	6:G:36:LYS:HA	1.91	0.52
17:R:44:LEU:HG	17:R:50:ILE:HA	1.92	0.52
3:D:76:ARG:O	3:D:80:GLU:HG2	2.10	0.52
20:A:1413:A:H61	20:A:1487:G:H1	0.72	0.52
20:A:1360:A:H2'	20:A:1361:G:O4'	2.08	0.52
20:A:308:C:H2'	20:A:309:G:C8	2.45	0.52
20:A:1016:A:O5'	20:A:1016:A:H8	1.93	0.52
20:A:116:A:H2'	20:A:117:G:O4'	2.09	0.52
6:G:74:GLU:HG2	6:G:91:VAL:HG22	1.92	0.52
21:W:72:C:H2'	21:W:73:A:O4'	2.10	0.52
1:B:54:THR:O	1:B:58:ILE:HG12	2.10	0.52
20:A:1281:U:H5'	20:A:1282:C:C5	2.38	0.52
20:A:68(F):C:H2'	20:A:68(G):G:H8	1.74	0.52
2:C:131:ARG:NH2	2:C:166:GLU:OE2	2.41	0.52
4:E:35:GLY:HA3	4:E:112:LEU:HD22	1.92	0.52
20:A:1343:G:H2'	20:A:1344:C:C6	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:75:THR:HB	4:E:117:ASP:O	2.08	0.52
7:H:21:LYS:O	7:H:23:SER:N	2.43	0.52
14:O:18:PHE:O	14:O:20:GLY:N	2.43	0.52
6:G:69:VAL:HA	6:G:138:LYS:HD2	1.90	0.52
20:A:1487:G:H2'	20:A:1488:G:H8	1.75	0.52
11:L:102:ARG:HB3	11:L:109:GLY:H	1.75	0.52
9:J:49:VAL:HG22	9:J:50:ILE:H	1.75	0.52
6:G:34:GLY:HA3	20:A:1350:A:C2	2.45	0.52
20:A:1324:A:H2'	20:A:1325:C:H6	1.75	0.52
17:R:65:ILE:O	17:R:69:THR:OG1	2.27	0.52
20:A:1440(K):G:H2'	20:A:1440(L):G:O4'	2.09	0.52
23:Y:256:THR:O	23:Y:258:VAL:HG23	2.10	0.52
23:Y:496:LYS:HG2	23:Y:498:ILE:HG23	1.92	0.52
19:T:59:ALA:O	19:T:63:ILE:HG13	2.09	0.52
23:Y:546:ILE:HA	23:Y:590:ILE:HG13	1.91	0.52
23:Y:616:TYR:CG	23:Y:663:THR:HA	2.45	0.52
20:A:488:C:H2'	20:A:489:C:C6	2.45	0.52
14:O:50:HIS:ND1	20:A:764:C:H5''	2.25	0.52
3:D:115:ARG:HB3	20:A:407:G:H5''	1.90	0.51
20:A:1178:G:N1	20:A:1181:G:OP2	2.42	0.51
20:A:935:A:H2'	20:A:936:C:C6	2.45	0.51
16:Q:83:ASP:N	16:Q:83:ASP:OD1	2.42	0.51
2:C:175:LEU:HD23	2:C:175:LEU:H	1.74	0.51
21:W:57:G:H2'	21:W:57:G:N3	2.26	0.51
20:A:296:U:H2'	20:A:297:G:C8	2.45	0.51
23:Y:29:THR:HA	23:Y:32:ILE:HB	1.93	0.51
20:A:1238:A:N3	20:A:1238:A:H2'	2.26	0.51
20:A:232:G:H1'	20:A:262:A:N1	2.25	0.51
18:S:46:GLY:HA2	18:S:62:ILE:HG23	1.92	0.51
4:E:98:THR:OG1	20:A:6:G:N2	2.28	0.51
1:B:184:VAL:HB	1:B:198:ASP:H	1.75	0.51
14:O:79:ARG:HA	14:O:82:ILE:HG22	1.91	0.51
7:H:26:VAL:HG22	7:H:32:LYS:NZ	2.25	0.51
20:A:1202:G:H2'	20:A:1203:C:H5'	1.93	0.51
23:Y:408:VAL:HG23	23:Y:409:ILE:HG12	1.93	0.51
20:A:612:C:H2'	20:A:613:C:H6	1.75	0.51
7:H:6:ILE:H	7:H:6:ILE:HD12	1.74	0.51
20:A:370:C:H42	20:A:391:G:H1	1.57	0.51
5:F:61:LEU:HB2	5:F:63:TYR:HE2	1.76	0.51
12:M:37:THR:HB	12:M:56:LEU:HA	1.93	0.51
20:A:1478:C:H2'	20:A:1479:C:C6	2.45	0.51
3:D:13:ARG:HG3	3:D:40:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:59:GLU:HG2	1:B:225:ALA:HB2	1.92	0.51
3:D:101:LEU:HD22	3:D:138:TYR:CD2	2.45	0.51
10:K:120:ARG:HH11	10:K:126:ARG:HH12	1.59	0.51
1:B:78:GLN:O	1:B:81:VAL:HG22	2.11	0.51
23:Y:422:GLU:O	23:Y:425:SER:HB2	2.10	0.51
2:C:7:PRO:HG2	2:C:201:TYR:HE2	1.76	0.51
20:A:1044:A:C5	20:A:1045:C:H1'	2.45	0.51
23:Y:544:LYS:HB3	23:Y:583:LYS:HE3	1.93	0.51
14:O:64:ARG:HH21	20:A:581:G:H4'	1.74	0.51
20:A:120:A:H2'	20:A:122:G:C8	2.46	0.51
9:J:87:THR:O	9:J:89:ASP:N	2.44	0.51
3:D:91:SER:HA	3:D:94:LEU:HD12	1.91	0.51
20:A:767:A:H2'	20:A:768:A:O4'	2.08	0.51
20:A:584:G:H2'	20:A:585:G:H8	1.74	0.51
23:Y:617:MET:HG2	23:Y:621:ILE:HD13	1.92	0.51
8:I:124:GLN:NE2	20:A:1232:U:OP1	2.42	0.51
6:G:46:ALA:O	6:G:50:ILE:HG13	2.11	0.51
19:T:73:HIS:C	19:T:74:LYS:HD3	2.31	0.51
1:B:162:ILE:HG13	1:B:185:ILE:O	2.11	0.51
3:D:57:ARG:NH2	4:E:107:ARG:HH21	2.02	0.51
11:L:49:ASN:HD21	20:A:528:C:H42	1.59	0.51
3:D:11:LEU:HB3	3:D:66:ARG:NH1	2.26	0.51
21:W:39:U:H2'	21:W:40:G:C8	2.43	0.51
1:B:49:GLU:O	1:B:52:GLU:HB3	2.11	0.51
20:A:368:U:C5	23:Y:354:ARG:HD3	2.46	0.51
20:A:1157:A:H61	20:A:1178:G:H1'	1.76	0.51
6:G:15:ASP:OD1	6:G:18:TYR:HB2	2.11	0.51
2:C:156:ARG:N	2:C:196:LEU:HD12	2.25	0.51
23:Y:197:ARG:HG3	23:Y:198:GLU:H	1.75	0.51
4:E:40:ARG:HE	4:E:66:MET:HE2	1.75	0.51
16:Q:97:SER:OG	16:Q:97:SER:O	2.26	0.51
1:B:97:TRP:HZ2	1:B:176:GLU:HG3	1.75	0.51
11:L:69:TYR:CG	11:L:70:ILE:N	2.77	0.51
13:N:23:ARG:HA	13:N:29:ARG:O	2.11	0.51
14:O:29:VAL:HG11	14:O:81:LEU:HD21	1.92	0.51
20:A:383:A:O5'	20:A:383:A:H8	1.94	0.51
5:F:9:VAL:HB	5:F:87:ARG:HB2	1.93	0.51
3:D:35:ARG:HD3	20:A:412:A:H2	1.76	0.51
23:Y:614:GLU:HA	23:Y:617:MET:HB3	1.93	0.51
13:N:48:ALA:HB2	13:N:53:LEU:HD12	1.93	0.51
20:A:1081:G:H2'	20:A:1082:G:C8	2.46	0.51
8:I:39:GLY:HA3	20:A:1291:G:H4'	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:271:C:H2'	20:A:272:C:O4'	2.10	0.51
20:A:280:C:H3'	20:A:281:G:C5'	2.38	0.51
21:W:1:G:N2	21:W:73:A:O2'	2.44	0.51
8:I:50:LEU:HB3	8:I:56:LEU:HA	1.93	0.51
20:A:1479:C:H2'	20:A:1480:G:H8	1.76	0.50
23:Y:8:ASP:HB3	23:Y:11:ARG:HG2	1.93	0.50
23:Y:20:HIS:CG	23:Y:21:ILE:H	2.27	0.50
20:A:1428:A:H2'	20:A:1429:C:O4'	2.11	0.50
20:A:255:G:H2'	20:A:256:U:C6	2.46	0.50
20:A:255:G:H2'	20:A:256:U:H6	1.76	0.50
19:T:17:ARG:HH12	20:A:102:G:H5''	1.76	0.50
20:A:643:C:H2'	20:A:644:G:H8	1.76	0.50
13:N:4:LYS:HG2	20:A:994:A:C2	2.46	0.50
20:A:1381:U:H5'	20:A:1382:C:OP2	2.11	0.50
20:A:1077:G:N2	20:A:1079:G:H3'	2.26	0.50
18:S:4:SER:O	20:A:1314:C:N4	2.44	0.50
20:A:1422:G:H2'	20:A:1423:G:C8	2.47	0.50
4:E:32:VAL:HG21	4:E:59:GLY:HA2	1.93	0.50
20:A:1284:C:OP2	20:A:1285:A:O2'	2.23	0.50
20:A:581:G:N2	20:A:760:G:N7	2.58	0.50
14:O:22:THR:HB	20:A:658:G:H4'	1.93	0.50
17:R:81:PHE:HB3	20:A:718:G:H1	1.77	0.50
20:A:399:G:H2'	20:A:400:C:C6	2.47	0.50
20:A:1486:G:H2'	20:A:1487:G:O4'	2.11	0.50
20:A:112:G:H2'	20:A:113:G:H8	1.77	0.50
21:W:18:G:O2'	21:W:57:G:N2	2.44	0.50
10:K:120:ARG:H	10:K:121:PRO:HD3	1.76	0.50
14:O:8:LYS:HG3	14:O:31:LEU:HD21	1.93	0.50
20:A:975:A:H2	20:A:1357:A:HO2'	1.58	0.50
23:Y:5:VAL:O	23:Y:7:TYR:N	2.45	0.50
20:A:1051:C:H2'	20:A:1052:U:C6	2.46	0.50
7:H:85:ARG:NH1	7:H:134:ILE:O	2.44	0.50
2:C:147:LYS:HB2	2:C:203:PHE:CE2	2.46	0.50
20:A:33:A:H2'	20:A:34:C:C6	2.47	0.50
20:A:68(P):C:H2'	20:A:68(Q):U:H6	1.77	0.50
20:A:745:C:H5''	20:A:851:G:H1'	1.92	0.50
8:I:107:ARG:NH2	20:A:1346:A:N3	2.58	0.50
7:H:121:ASP:OD1	7:H:121:ASP:N	2.39	0.50
15:P:21:VAL:HG11	15:P:59:TRP:CE2	2.46	0.50
21:W:16:U:H5'	21:W:59:A:N1	2.27	0.50
23:Y:627:ARG:NH2	23:Y:658:ASP:OD1	2.44	0.50
3:D:127:THR:HG23	3:D:147:ALA:HB3	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:66:VAL:HG12	6:G:70:LYS:HE2	1.94	0.50
20:A:769:G:H4'	20:A:1513:A:H4'	1.94	0.50
16:Q:68:ARG:HH12	20:A:277:C:H5'	1.77	0.50
23:Y:394:ALA:O	23:Y:396:ARG:N	2.45	0.50
20:A:1391:U:H2'	20:A:1392:G:H8	1.76	0.50
16:Q:64:PRO:HB3	16:Q:70:ARG:HH12	1.75	0.50
20:A:540:G:H2'	20:A:541:G:O4'	2.11	0.50
4:E:17:ALA:O	20:A:15:G:N2	2.32	0.50
23:Y:317:MET:HB3	23:Y:325:LEU:HB2	1.93	0.50
3:D:15:GLU:OE1	3:D:63:LYS:HA	2.12	0.50
12:M:107:ALA:H	12:M:108:ARG:HD2	1.77	0.50
18:S:36:ARG:HH12	18:S:75:ALA:HB3	1.77	0.50
20:A:68(H):G:N2	20:A:68(R):C:N3	2.57	0.50
16:Q:44:ALA:HB2	16:Q:59:ILE:HD11	1.94	0.50
20:A:570:G:O6	20:A:865:A:N6	2.45	0.50
20:A:1288:A:N1	20:A:1371:G:H1'	2.26	0.50
4:E:91:LEU:HD13	4:E:118:ILE:HG12	1.92	0.50
19:T:74:LYS:HG2	19:T:75:ASN:H	1.76	0.50
23:Y:556:ILE:HD13	23:Y:556:ILE:H	1.77	0.50
20:A:1012:U:H2'	20:A:1013:G:C8	2.47	0.50
3:D:25:ARG:HG3	3:D:30:LYS:HE3	1.92	0.50
20:A:406:G:H2'	20:A:407:G:C8	2.47	0.50
1:B:88:ALA:HB2	1:B:219:VAL:HG13	1.93	0.50
18:S:36:ARG:NH2	18:S:75:ALA:O	2.45	0.50
23:Y:243:VAL:HA	23:Y:279:TYR:CE1	2.47	0.50
13:N:4:LYS:NZ	20:A:1047:G:OP1	2.32	0.50
20:A:42:G:H2'	20:A:43:C:C6	2.47	0.50
23:Y:554:PRO:HG3	23:Y:594:VAL:HG12	1.93	0.50
3:D:175:SER:HB2	3:D:186:LEU:HD11	1.94	0.50
20:A:1280:A:O2'	20:A:1281:U:OP1	2.26	0.50
12:M:105:THR:HG22	20:A:1229:A:N6	2.26	0.50
20:A:612:C:H42	20:A:628:G:H1	1.60	0.50
20:A:901:A:H8	20:A:901:A:O5'	1.95	0.50
10:K:44:SER:H	10:K:47:VAL:HG21	1.75	0.50
3:D:134:ASP:N	3:D:134:ASP:OD2	2.44	0.50
14:O:24:SER:O	14:O:28:GLN:NE2	2.45	0.50
23:Y:257:PRO:O	23:Y:259:PHE:N	2.40	0.49
23:Y:607:ARG:HA	23:Y:645:ALA:O	2.11	0.49
20:A:976:G:OP2	20:A:1358:U:O2'	2.26	0.49
20:A:859:A:H3'	20:A:860:A:H8	1.77	0.49
8:I:97:LYS:HD3	20:A:1178:G:N7	2.27	0.49
20:A:745:C:H2'	20:A:746:A:C8	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1019:C:H2'	20:A:1020:U:O4'	2.12	0.49
16:Q:12:SER:HB2	16:Q:14:LYS:HD2	1.94	0.49
5:F:75:LEU:O	5:F:79:LEU:HG	2.11	0.49
23:Y:265:LYS:O	23:Y:267:LYS:N	2.45	0.49
20:A:671:G:H2'	20:A:672:U:C6	2.47	0.49
23:Y:342:TYR:HB2	23:Y:349:LYS:HA	1.94	0.49
23:Y:219:VAL:HG11	23:Y:255:ILE:HD11	1.92	0.49
20:A:424:G:H2'	20:A:425:G:H8	1.77	0.49
23:Y:569:ASP:OD1	23:Y:570:GLY:N	2.37	0.49
10:K:16:SER:HA	10:K:79:SER:O	2.12	0.49
23:Y:111:SER:HB2	23:Y:141:LYS:HG2	1.94	0.49
3:D:33:MET:O	3:D:36:ARG:N	2.46	0.49
20:A:1065:U:OP2	20:A:1190:G:N2	2.30	0.49
1:B:102:LEU:O	1:B:180:LEU:HD11	2.11	0.49
11:L:71:PRO:HD3	11:L:100:ILE:HB	1.94	0.49
20:A:1127:G:N2	20:A:1147:C:H41	2.09	0.49
12:M:116:THR:HA	20:A:1228:C:H4'	1.93	0.49
23:Y:316:ILE:HD11	23:Y:385:THR:HB	1.94	0.49
21:W:29:U:H2'	21:W:30:C:O4'	2.12	0.49
3:D:15:GLU:OE1	3:D:19:LEU:HD21	2.12	0.49
12:M:20:THR:C	12:M:22:ILE:H	2.15	0.49
18:S:78:ARG:NH1	20:A:1225:A:H5'	2.26	0.49
2:C:8:ILE:HD12	2:C:16:ARG:HH12	1.76	0.49
20:A:927:G:O6	20:A:1390:U:O2	2.30	0.49
20:A:218:C:O2'	20:A:458(C):G:N2	2.44	0.49
20:A:999:U:O4	20:A:1000:A:N6	2.45	0.49
23:Y:127:LYS:HA	23:Y:127:LYS:HE2	1.95	0.49
11:L:53:ARG:HB3	11:L:93:LEU:HD13	1.93	0.49
23:Y:338:GLY:O	23:Y:351:ARG:NH2	2.45	0.49
21:W:12:U:H3	21:W:23:A:N6	2.07	0.49
20:A:545:C:O2'	20:A:549:C:OP1	2.30	0.49
20:A:299:G:H2'	20:A:300:A:C8	2.48	0.49
10:K:29:ILE:HD12	20:A:706:A:H1'	1.94	0.49
23:Y:341:VAL:N	23:Y:350:GLU:O	2.34	0.49
5:F:98:LEU:HA	17:R:31:LEU:H	1.77	0.49
23:Y:509:HIS:CE1	23:Y:511:LYS:HE3	2.47	0.49
16:Q:90:ILE:HG21	20:A:583:A:H5'	1.94	0.49
14:O:5:LYS:HD3	14:O:5:LYS:H	1.78	0.49
20:A:823:G:H1	20:A:877:C:H42	1.61	0.49
10:K:124:LYS:NZ	20:A:692:U:OP1	2.28	0.49
20:A:152:A:H3'	20:A:153:C:H6	1.77	0.49
20:A:1468:A:H2'	20:A:1469:G:O4'	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:64:G:H4'	20:A:65:U:H3'	1.93	0.49
20:A:428:G:H1'	20:A:430:A:C8	2.48	0.49
1:B:170:GLU:HA	1:B:173:ALA:HB3	1.95	0.49
13:N:17:LYS:HG2	20:A:1317:C:OP1	2.13	0.49
20:A:781:A:H1'	20:A:1523:G:H1'	1.94	0.49
20:A:949:A:H2'	20:A:950:U:C6	2.47	0.49
15:P:5:ARG:HB2	20:A:376:G:H5''	1.95	0.49
2:C:172:ARG:NH2	20:A:1107:C:OP1	2.41	0.49
23:Y:133:ILE:HG22	23:Y:257:PRO:HB2	1.94	0.49
7:H:9:MET:O	7:H:13:ILE:HG12	2.13	0.49
6:G:26:PHE:CE2	6:G:30:ILE:HD11	2.47	0.49
1:B:55:PHE:HE1	1:B:218:ALA:HA	1.77	0.49
9:J:34:VAL:HG22	9:J:74:ILE:HG22	1.95	0.49
23:Y:659:LEU:O	23:Y:661:SER:N	2.45	0.49
20:A:68(V):G:C2	20:A:68(W):G:H1'	2.47	0.49
3:D:26:CYS:HA	3:D:30:LYS:O	2.13	0.49
20:A:17:U:H2'	20:A:18:C:C6	2.47	0.49
20:A:1399:C:C2	20:A:1502:A:N6	2.81	0.49
12:M:78:ILE:HD13	12:M:81:LEU:HD22	1.95	0.49
21:W:19:G:H1	21:W:56:C:H42	1.59	0.49
15:P:8:ARG:HB2	15:P:17:TYR:CE2	2.47	0.49
20:A:162:A:H3'	20:A:163:C:O4'	2.12	0.49
20:A:1183:A:O2'	20:A:1184:G:H5''	2.13	0.49
5:F:70:ASP:O	5:F:73:ASN:ND2	2.45	0.49
20:A:1487:G:H2'	20:A:1488:G:C8	2.48	0.49
23:Y:314:PHE:CZ	23:Y:329:ARG:HB3	2.39	0.49
20:A:1115:C:H2'	20:A:1116:C:H5'	1.95	0.49
6:G:15:ASP:HB2	6:G:20:ASP:O	2.12	0.49
20:A:1039:C:H2'	20:A:1040:U:C6	2.48	0.49
20:A:163:C:H2'	20:A:164:U:H6	1.78	0.49
7:H:34:GLU:O	7:H:38:ILE:HG12	2.11	0.49
20:A:669:U:H2'	20:A:670:G:C8	2.47	0.49
20:A:817:C:O2'	20:A:1527:C:O3'	2.31	0.49
2:C:8:ILE:HD12	2:C:16:ARG:NH1	2.28	0.49
20:A:966:G:H1'	21:W:34:C:H4'	1.94	0.49
20:A:1461:G:H2'	20:A:1462:G:C8	2.47	0.49
16:Q:12:SER:HA	16:Q:14:LYS:HZ2	1.78	0.49
2:C:6:HIS:ND1	13:N:49:HIS:HB3	2.27	0.49
11:L:43:VAL:HG12	11:L:44:THR:H	1.77	0.49
20:A:1394:A:H8	20:A:1501:C:HO2'	1.61	0.48
1:B:77:ALA:O	1:B:81:VAL:N	2.35	0.48
20:A:441:A:H62	20:A:493:G:N2	2.07	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:89:ASN:HB3	8:I:92:TYR:CD1	2.48	0.48
20:A:569:C:H42	20:A:881:G:H1	1.61	0.48
20:A:1048:G:H2'	20:A:1050:G:C8	2.48	0.48
22:V:12:A:H2'	22:V:13:A:H5'	1.95	0.48
20:A:488:C:H2'	20:A:489:C:H6	1.78	0.48
2:C:154:SER:HA	2:C:165:THR:HA	1.94	0.48
20:A:683:G:H2'	20:A:684:A:C8	2.48	0.48
10:K:108:ILE:HD13	17:R:87:ARG:HA	1.95	0.48
13:N:6:LEU:HD13	13:N:23:ARG:HH22	1.79	0.48
11:L:80:HIS:O	11:L:82:VAL:N	2.40	0.48
20:A:1139:G:N2	20:A:1142:G:O6	2.46	0.48
5:F:48:LEU:N	5:F:56:PRO:O	2.38	0.48
8:I:25:LYS:O	8:I:25:LYS:HG3	2.13	0.48
20:A:284:G:H2'	20:A:285:G:C8	2.47	0.48
20:A:1260:C:H42	20:A:1274:G:H1	1.60	0.48
4:E:75:THR:OG1	4:E:76:ILE:N	2.45	0.48
8:I:25:LYS:O	8:I:61:ALA:N	2.41	0.48
15:P:2:VAL:HA	15:P:23:ASP:HA	1.94	0.48
6:G:108:ALA:HB1	6:G:120:ILE:HD13	1.95	0.48
20:A:571:U:H5''	20:A:819:A:C5	2.48	0.48
20:A:1090:U:H2'	20:A:1091:U:C6	2.48	0.48
22:V:18:G:H5'	22:V:19:G:OP1	2.13	0.48
21:W:15:G:N2	21:W:48:C:N4	2.16	0.48
20:A:27:G:H2'	20:A:28:G:C8	2.49	0.48
3:D:175:SER:O	3:D:183:GLY:HA2	2.14	0.48
11:L:76:ASN:ND2	11:L:77:LEU:H	2.10	0.48
11:L:115:LYS:O	11:L:117:ARG:N	2.39	0.48
6:G:7:ALA:HB3	20:A:1378:C:OP1	2.13	0.48
23:Y:606:MET:HG2	23:Y:673:PHE:HA	1.95	0.48
20:A:120:A:H2'	20:A:122:G:N7	2.28	0.48
9:J:36:GLY:HA3	20:A:1123:A:H4'	1.95	0.48
11:L:123:LYS:HD2	20:A:37:U:P	2.53	0.48
15:P:16:HIS:CE1	15:P:38:TYR:HB2	2.48	0.48
14:O:55:GLY:O	14:O:59:MET:HG3	2.12	0.48
20:A:410:G:H2'	20:A:429:U:C5	2.48	0.48
20:A:766:A:H2'	20:A:767:A:O4'	2.13	0.48
23:Y:100:VAL:HG21	23:Y:314:PHE:HZ	1.78	0.48
20:A:68(H):G:N3	20:A:68(H):G:H2'	2.28	0.48
20:A:1251:A:N3	20:A:1369:C:O2'	2.32	0.48
14:O:10:LYS:O	14:O:14:GLU:HB2	2.13	0.48
16:Q:86:GLU:O	16:Q:90:ILE:HG13	2.14	0.48
4:E:146:ALA:O	4:E:150:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:43:ALA:HA	8:I:74:ILE:HG21	1.95	0.48
8:I:117:HIS:HE1	8:I:123:PRO:HB3	1.78	0.48
17:R:36:ASN:HB3	17:R:39:VAL:HB	1.96	0.48
2:C:24:ALA:HB3	9:J:11:PHE:HZ	1.77	0.48
20:A:1394:A:N7	20:A:1501:C:H4'	2.28	0.48
20:A:1218:C:H2'	20:A:1219:U:H6	1.78	0.48
23:Y:96:ARG:HA	23:Y:99:ARG:CB	2.43	0.48
8:I:107:ARG:NH2	20:A:1346:A:H1'	2.27	0.48
20:A:766:A:H61	20:A:1511:G:H1'	1.79	0.48
20:A:553:A:H2'	20:A:554:C:H6	1.79	0.48
6:G:34:GLY:HA3	20:A:1350:A:H2	1.77	0.48
16:Q:69:LYS:HG3	20:A:254:G:H5''	1.96	0.48
2:C:157:ILE:HD13	2:C:164:ARG:NE	2.27	0.48
8:I:93:ARG:NE	8:I:102:LEU:HD11	2.29	0.48
20:A:1419:G:H2'	20:A:1420:C:H6	1.78	0.48
20:A:131:C:H2'	20:A:132:C:H6	1.78	0.48
20:A:590:C:H2'	20:A:591:U:C6	2.48	0.48
23:Y:199:ILE:HG12	23:Y:200:PRO:O	2.13	0.48
20:A:62:U:H2'	20:A:63:C:C6	2.49	0.48
20:A:1412:C:H42	20:A:1488:G:H1	1.61	0.48
23:Y:137:ASN:ND2	23:Y:138:LYS:N	2.47	0.48
11:L:45:PRO:HD2	11:L:49:ASN:HB2	1.95	0.48
11:L:82:VAL:HG12	11:L:82:VAL:O	2.14	0.48
20:A:1017:G:H2'	20:A:1018:C:C6	2.49	0.48
20:A:411:A:O2'	20:A:413:G:OP1	2.27	0.48
12:M:39:ILE:HD12	12:M:56:LEU:HG	1.96	0.48
10:K:27:ASN:ND2	10:K:55:LYS:HD2	2.28	0.48
7:H:32:LYS:O	7:H:36:LEU:HG	2.13	0.48
20:A:606:G:H3'	20:A:607:A:H5'	1.95	0.48
5:F:1:MET:HA	5:F:68:PRO:HA	1.96	0.48
2:C:5:ILE:HG22	20:A:1190:G:OP1	2.14	0.48
20:A:555:C:H2'	20:A:556:C:C6	2.49	0.48
20:A:973:G:C8	20:A:974:A:H2'	2.48	0.48
19:T:49:ALA:O	19:T:52:ALA:N	2.46	0.48
20:A:1369:C:H2'	20:A:1370:G:O4'	2.14	0.48
20:A:757:U:O2'	20:A:879:C:O2	2.32	0.48
11:L:5:PRO:HG2	11:L:15:ARG:NH2	2.28	0.48
7:H:88:LYS:C	7:H:90:GLY:H	2.17	0.48
23:Y:187:THR:HG22	23:Y:198:GLU:HA	1.95	0.48
5:F:51:PRO:HA	5:F:56:PRO:HA	1.95	0.48
5:F:44:GLY:HA2	5:F:59:TYR:CE1	2.49	0.48
6:G:150:ALA:HB1	10:K:93:GLN:HE22	1.79	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:W:52:G:H1	21:W:62:C:H42	1.62	0.48
23:Y:137:ASN:HD22	23:Y:262:SER:HA	1.78	0.47
23:Y:631:ILE:HG22	23:Y:632:LEU:N	2.29	0.47
3:D:62:GLN:NE2	20:A:544:G:OP1	2.45	0.47
7:H:109:ILE:HG13	7:H:120:THR:HB	1.96	0.47
7:H:9:MET:HE2	7:H:32:LYS:HG2	1.96	0.47
15:P:70:ALA:O	15:P:73:LEU:N	2.47	0.47
2:C:87:LEU:O	2:C:91:LEU:HG	2.14	0.47
9:J:35:SER:HB3	9:J:73:ASP:HB2	1.96	0.47
3:D:73:ARG:HB2	20:A:546:G:OP1	2.14	0.47
20:A:124:G:H4'	20:A:291:C:O2'	2.14	0.47
20:A:125:U:H2'	20:A:126:G:C8	2.49	0.47
1:B:171:ALA:HA	1:B:174:VAL:CB	2.39	0.47
1:B:97:TRP:CZ2	1:B:176:GLU:HG3	2.48	0.47
8:I:22:GLY:HA3	8:I:60:ASP:CG	2.34	0.47
8:I:33:PHE:HE1	8:I:43:ALA:HB1	1.79	0.47
15:P:2:VAL:HG11	20:A:228:A:O2'	2.14	0.47
8:I:117:HIS:CE1	8:I:123:PRO:HB3	2.49	0.47
2:C:24:ALA:HB1	2:C:29:TYR:HB2	1.95	0.47
6:G:139:GLU:O	6:G:143:ARG:HG3	2.14	0.47
7:H:107:LEU:HD23	7:H:107:LEU:H	1.79	0.47
11:L:36:VAL:H	11:L:58:VAL:HA	1.78	0.47
20:A:436:C:H2'	20:A:437:U:O4'	2.15	0.47
20:A:558:G:C8	20:A:559:A:H2'	2.50	0.47
20:A:1362:C:H2'	20:A:1362(A):C:H5''	1.97	0.47
4:E:18:ARG:HA	20:A:15:G:N2	2.28	0.47
16:Q:61:GLU:HB2	16:Q:71:PHE:CE1	2.50	0.47
19:T:22:ARG:HB3	20:A:324:G:OP1	2.14	0.47
19:T:12:ALA:O	19:T:15:ARG:HB2	2.14	0.47
23:Y:420:ASP:O	23:Y:423:LYS:HB3	2.14	0.47
23:Y:453:GLY:HA3	23:Y:459:LEU:HD11	1.97	0.47
20:A:59:A:H1'	20:A:354:G:N2	2.28	0.47
20:A:112:G:H2'	20:A:113:G:C8	2.49	0.47
6:G:88:PRO:HD2	6:G:151:TYR:HB2	1.95	0.47
14:O:56:LEU:O	14:O:60:VAL:HG23	2.15	0.47
1:B:81:VAL:HG12	1:B:215:LEU:HD11	1.96	0.47
20:A:427:U:O2'	20:A:541:G:OP1	2.32	0.47
20:A:945:G:C2	20:A:946:A:C8	3.02	0.47
20:A:68(I):G:C2	20:A:68(R):C:H1'	2.50	0.47
20:A:1114:C:H2'	20:A:1115:C:C6	2.49	0.47
3:D:157:LEU:HA	3:D:160:GLN:HB2	1.95	0.47
20:A:186(N):U:H2'	20:A:186(O):G:C8	2.49	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:344:A:H8	20:A:344:A:P	2.38	0.47
3:D:8:VAL:HG11	3:D:115:ARG:HD3	1.94	0.47
20:A:27:G:H2'	20:A:28:G:H8	1.80	0.47
11:L:49:ASN:ND2	20:A:529:G:O6	2.47	0.47
14:O:12:ILE:HG23	14:O:27:VAL:HG13	1.96	0.47
13:N:33:VAL:HA	13:N:40:CYS:HA	1.95	0.47
1:B:35:GLU:HG3	1:B:40:HIS:CG	2.50	0.47
20:A:525:C:H2'	20:A:526:C:C6	2.49	0.47
16:Q:5:VAL:HG12	16:Q:59:ILE:O	2.14	0.47
20:A:434:U:H2'	20:A:435:C:C6	2.49	0.47
23:Y:121:VAL:O	23:Y:125:ALA:HB2	2.15	0.47
9:J:28:ARG:NH2	9:J:34:VAL:O	2.48	0.47
21:W:58:A:O2'	21:W:60:U:O5'	2.32	0.47
8:I:2:GLU:N	8:I:88:TYR:OH	2.45	0.47
25:Y:701:FUA:H122	25:Y:701:FUA:H231	1.95	0.47
20:A:937:A:O2'	20:A:1378:C:N4	2.47	0.47
5:F:46:ARG:HB3	5:F:60:PHE:CE1	2.49	0.47
2:C:22:TRP:HA	9:J:93:GLY:HA2	1.97	0.47
7:H:12:ARG:NH1	7:H:26:VAL:HG23	2.30	0.47
23:Y:400:GLU:O	23:Y:402:ILE:HG13	2.15	0.47
19:T:15:ARG:NH2	20:A:108:G:N3	2.63	0.47
20:A:983:A:H2	20:A:984:C:H5	1.63	0.47
14:O:33:THR:OG1	14:O:85:LEU:HD21	2.15	0.47
23:Y:25:LYS:HG3	26:Y:702:GDP:O2B	2.15	0.47
20:A:114:U:H3	20:A:313:A:H2	1.60	0.47
11:L:85:ILE:HD12	11:L:98:TYR:CB	2.44	0.47
3:D:26:CYS:HA	3:D:31:CYS:HA	1.97	0.47
20:A:1504:G:H4'	20:A:1505:G:C5'	2.44	0.47
13:N:45:ARG:NH2	20:A:1059:C:O3'	2.48	0.47
11:L:80:HIS:NE2	23:Y:425:SER:HB3	2.29	0.47
20:A:1414:U:H2'	20:A:1415:G:C8	2.43	0.47
12:M:108:ARG:HB2	20:A:948:C:OP2	2.15	0.47
12:M:91:ARG:HH21	12:M:96:LEU:HD13	1.79	0.47
20:A:137:C:N4	20:A:226:G:H1	2.12	0.47
9:J:92:THR:OG1	9:J:93:GLY:N	2.46	0.47
8:I:70:LYS:O	8:I:73:GLN:HB2	2.14	0.47
15:P:6:LEU:HG	15:P:19:ILE:HD13	1.96	0.47
4:E:30:ALA:O	4:E:45:PHE:HA	2.15	0.47
2:C:40:ARG:HH12	13:N:52:GLN:HB3	1.80	0.47
1:B:7:VAL:HA	1:B:11:LEU:HD12	1.96	0.47
11:L:52:LEU:HG	11:L:54:LYS:NZ	2.29	0.47
3:D:172:PRO:HB2	3:D:187:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:K:114:VAL:HG13	20:A:675:A:O2'	2.15	0.47
20:A:663:A:N6	20:A:742:G:H1	2.12	0.47
20:A:68(P):C:H2'	20:A:68(Q):U:C6	2.50	0.47
23:Y:291:GLY:HA2	23:Y:400:GLU:HB2	1.97	0.47
19:T:76:ALA:HB2	20:A:262:A:H5''	1.95	0.47
20:A:1326:C:H2'	20:A:1327:C:H6	1.78	0.47
23:Y:520:GLY:N	23:Y:562:ASP:OD1	2.47	0.47
20:A:1353:G:H2'	20:A:1354:C:H6	1.80	0.47
23:Y:455:GLY:O	23:Y:458:HIS:HB3	2.15	0.47
2:C:72:LYS:HE3	2:C:75:VAL:H	1.79	0.47
20:A:627:G:H2'	20:A:628:G:C8	2.49	0.47
20:A:862:C:H42	20:A:867:G:H1	1.61	0.47
16:Q:57:VAL:HG23	16:Q:59:ILE:HG13	1.96	0.47
20:A:1230:C:H2'	20:A:1231:G:C8	2.49	0.47
7:H:9:MET:HB2	7:H:26:VAL:HG21	1.97	0.47
20:A:1534:A:H2'	20:A:1535:C:H6	1.80	0.47
20:A:1328:C:H2'	20:A:1329:A:O4'	2.14	0.47
23:Y:438:PHE:HB2	23:Y:452:SER:O	2.15	0.47
20:A:259:G:H2'	20:A:260:G:C8	2.50	0.47
19:T:16:HIS:O	19:T:20:LEU:HG	2.15	0.47
20:A:68(O):A:C8	20:A:68(P):C:H1'	2.50	0.47
18:S:64:GLU:O	18:S:66:MET:N	2.43	0.47
23:Y:416:LYS:HE2	23:Y:416:LYS:HB3	1.66	0.47
13:N:43:CYS:O	13:N:46:GLU:HG2	2.15	0.47
6:G:118:VAL:HG13	6:G:122:HIS:CE1	2.49	0.47
23:Y:475:ASN:N	23:Y:475:ASN:OD1	2.47	0.47
1:B:69:LEU:H	1:B:163:PHE:N	2.12	0.46
13:N:17:LYS:HD2	20:A:1316:G:H5''	1.97	0.46
12:M:125:ARG:HH12	20:A:953:G:H5'	1.80	0.46
4:E:126:ARG:HD3	20:A:10:A:OP2	2.16	0.46
20:A:1157:A:H4'	20:A:1158:C:O5'	2.16	0.46
20:A:971:G:N1	20:A:1363:A:OP2	2.44	0.46
12:M:14:ARG:HB2	12:M:17:VAL:HG23	1.97	0.46
2:C:35:GLU:O	2:C:39:ILE:HG13	2.15	0.46
20:A:694:A:H2'	20:A:695:A:O4'	2.15	0.46
23:Y:179:ASP:N	23:Y:184:LYS:O	2.36	0.46
20:A:175:C:H2'	20:A:176:C:H6	1.80	0.46
6:G:32:ARG:HG2	20:A:1240:U:C2	2.50	0.46
23:Y:615:GLU:HG2	23:Y:615:GLU:H	1.44	0.46
20:A:113:G:H2'	20:A:114:U:H6	1.79	0.46
11:L:36:VAL:O	11:L:37:CYS:HB3	2.15	0.46
11:L:38:THR:HG22	11:L:57:LYS:HB2	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:P:53:VAL:O	15:P:57:ARG:HD3	2.15	0.46
20:A:1376:U:H2'	20:A:1377:A:H8	1.78	0.46
2:C:163:ALA:CB	20:A:1056:U:H4'	2.44	0.46
9:J:91:PRO:HB2	9:J:94:VAL:HB	1.96	0.46
20:A:1401:G:H5''	22:V:22:A:N6	2.30	0.46
20:A:413:G:H1'	20:A:428:G:N2	2.30	0.46
1:B:70:PHE:O	1:B:93:VAL:N	2.48	0.46
8:I:118:LYS:O	8:I:120:ARG:N	2.48	0.46
20:A:976:G:H5'	20:A:1358:U:O2'	2.14	0.46
20:A:1304:G:H1'	20:A:1333:A:N6	2.30	0.46
12:M:96:LEU:HD11	20:A:1226:C:H5''	1.98	0.46
23:Y:238:THR:O	23:Y:241:GLU:HG2	2.16	0.46
20:A:614:A:H2'	20:A:615:C:C6	2.51	0.46
12:M:66:LEU:HB3	12:M:67:GLU:H	1.53	0.46
20:A:660:G:H2'	20:A:661:G:C8	2.51	0.46
1:B:113:HIS:O	1:B:117:GLU:HG2	2.16	0.46
20:A:405:U:H5''	20:A:406:G:O4'	2.15	0.46
14:O:48:LYS:HB3	20:A:668:G:H4'	1.96	0.46
23:Y:309:LEU:O	23:Y:394:ALA:HB1	2.16	0.46
23:Y:93:GLU:OE1	23:Y:97:SER:OG	2.32	0.46
23:Y:621:ILE:HD11	23:Y:643:ILE:HG12	1.96	0.46
23:Y:354:ARG:NH2	23:Y:378:VAL:HG21	2.31	0.46
23:Y:29:THR:HG22	23:Y:33:LEU:HD13	1.97	0.46
11:L:15:ARG:NH2	20:A:567:G:N7	2.63	0.46
15:P:8:ARG:HA	15:P:17:TYR:HA	1.97	0.46
14:O:50:HIS:CG	20:A:764:C:H5''	2.51	0.46
19:T:53:LEU:HA	19:T:56:MET:HB2	1.96	0.46
20:A:1501:C:OP1	20:A:1508:G:H4'	2.15	0.46
1:B:69:LEU:H	1:B:162:ILE:HA	1.81	0.46
1:B:77:ALA:O	1:B:81:VAL:HG13	2.15	0.46
11:L:71:PRO:HB2	11:L:102:ARG:NH1	2.24	0.46
13:N:29:ARG:NH2	20:A:974:A:OP2	2.47	0.46
12:M:115:LYS:N	20:A:1228:C:H5'	2.31	0.46
20:A:1339:A:H4'	21:W:40:G:O2'	2.15	0.46
20:A:745:C:H5''	20:A:851:G:O2'	2.15	0.46
1:B:113:HIS:O	1:B:116:GLU:HG2	2.15	0.46
6:G:38:LEU:O	6:G:42:ILE:HG12	2.15	0.46
19:T:62:LEU:HA	19:T:65:LYS:HG2	1.97	0.46
3:D:5:ILE:HD13	20:A:406:G:H4'	1.97	0.46
20:A:17:U:H2'	20:A:18:C:H6	1.80	0.46
20:A:1528:U:O2'	20:A:1530:G:H5'	2.16	0.46
1:B:173:ALA:O	1:B:176:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1356:G:H2'	20:A:1357:A:H8	1.75	0.46
20:A:1015:A:C6	20:A:1016:A:C6	3.03	0.46
13:N:61:TRP:CZ2	20:A:1368:G:H4'	2.48	0.46
20:A:590:C:H2'	20:A:591:U:H6	1.81	0.46
20:A:1239:A:H62	20:A:1299:A:H61	1.61	0.46
9:J:57:LYS:HE2	20:A:972:C:OP2	2.15	0.46
20:A:455:C:H2'	20:A:456:C:C6	2.51	0.46
20:A:14:U:O5'	20:A:14:U:H6	1.99	0.46
11:L:85:ILE:HD12	11:L:98:TYR:HB2	1.98	0.46
20:A:1440(J):C:H1'	20:A:1440(K):G:C2	2.51	0.46
7:H:19:VAL:HG21	20:A:827:U:H4'	1.98	0.46
16:Q:45:HIS:H	16:Q:72:ARG:CA	2.28	0.46
3:D:62:GLN:NE2	20:A:545:C:OP2	2.49	0.46
19:T:71:THR:HB	19:T:72:LEU:H	1.62	0.46
15:P:59:TRP:HA	15:P:62:VAL:HG22	1.98	0.46
23:Y:543:GLN:HA	23:Y:546:ILE:HD12	1.98	0.46
20:A:692:U:H2'	20:A:694:A:OP2	2.16	0.46
2:C:195:VAL:HG12	20:A:1057:G:H1'	1.98	0.46
20:A:371:G:H1	20:A:390:C:H42	1.64	0.46
20:A:687:A:C2	20:A:704:A:C6	3.04	0.46
20:A:1059:C:H2'	20:A:1060:C:O4'	2.16	0.46
11:L:124:LYS:O	11:L:126:LYS:N	2.49	0.46
23:Y:333:GLY:H	23:Y:371:ALA:CB	2.27	0.46
6:G:102:ARG:CZ	20:A:939:G:H5''	2.45	0.46
21:W:41:A:HO2'	21:W:42:U:P	2.38	0.46
20:A:949:A:O2'	20:A:971:G:O6	2.22	0.46
7:H:6:ILE:O	7:H:10:LEU:HG	2.15	0.46
12:M:23:TYR:CE2	20:A:1330:U:H4'	2.51	0.46
20:A:988:G:H2'	20:A:989:C:O4'	2.15	0.46
1:B:67:THR:HA	1:B:90:MET:SD	2.55	0.46
8:I:4:TYR:HB2	8:I:19:LEU:CB	2.39	0.46
2:C:72:LYS:HD2	2:C:73:PRO:HD2	1.97	0.46
20:A:722:A:H4'	20:A:723:U:C5	2.48	0.46
19:T:63:ILE:HG21	19:T:81:LYS:HG3	1.98	0.46
8:I:33:PHE:CE1	8:I:43:ALA:HB1	2.51	0.46
5:F:69:GLU:O	5:F:72:VAL:HG12	2.15	0.46
3:D:128:VAL:HA	3:D:145:GLU:O	2.16	0.46
23:Y:197:ARG:HA	23:Y:197:ARG:CZ	2.46	0.46
2:C:6:HIS:CG	13:N:49:HIS:HB3	2.51	0.46
23:Y:17:ILE:HA	23:Y:105:ILE:O	2.16	0.46
4:E:57:LYS:O	4:E:60:TYR:HB3	2.16	0.46
3:D:108:LEU:HD23	3:D:110:PHE:CZ	2.50	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:272:LEU:HD12	23:Y:275:ALA:HB3	1.97	0.46
20:A:1392:G:H2'	20:A:1393:U:C6	2.51	0.46
12:M:91:ARG:NH2	12:M:96:LEU:HB3	2.31	0.46
18:S:31:ILE:HD11	18:S:49:ILE:HG12	1.98	0.46
9:J:46:ARG:HD2	13:N:61:TRP:CZ3	2.50	0.46
20:A:186:C:H2'	20:A:186(A):C:O4'	2.16	0.46
23:Y:216:LEU:HD21	23:Y:242:LEU:HD22	1.98	0.46
5:F:50:TYR:CZ	17:R:77:GLY:HA2	2.51	0.46
2:C:51:GLY:C	2:C:115:LEU:HD21	2.36	0.46
2:C:71:ALA:HB2	2:C:115:LEU:HD22	1.98	0.46
1:B:160:ASP:HA	1:B:182:ILE:HD12	1.98	0.46
20:A:620:C:H2'	20:A:621:A:O4'	2.16	0.45
1:B:162:ILE:CG1	1:B:184:VAL:HA	2.46	0.45
8:I:16:ARG:HH12	20:A:1128:C:H4'	1.82	0.45
18:S:58:VAL:HG21	18:S:75:ALA:HB2	1.97	0.45
20:A:458(A):G:N2	20:A:458(E):A:H62	2.13	0.45
23:Y:301:ILE:HG21	23:Y:331:TYR:HB3	1.97	0.45
20:A:1252:A:H2'	20:A:1253:G:C8	2.51	0.45
20:A:242:C:H2'	20:A:245:C:C5	2.51	0.45
15:P:32:TYR:OH	20:A:608:A:H4'	2.16	0.45
1:B:236:TYR:HA	1:B:239:VAL:HB	1.97	0.45
10:K:108:ILE:HB	17:R:87:ARG:H	1.81	0.45
20:A:1149:C:O2'	20:A:1280:A:N1	2.50	0.45
20:A:947:G:H2'	20:A:948:C:O4'	2.17	0.45
20:A:418:C:N4	20:A:425:G:H1	2.13	0.45
10:K:51:LYS:HA	10:K:55:LYS:HG3	1.99	0.45
9:J:46:ARG:NH2	20:A:1253:G:OP1	2.42	0.45
10:K:41:THR:CG2	10:K:71:LYS:HD3	2.45	0.45
23:Y:115:GLU:N	23:Y:116:PRO:HD3	2.31	0.45
15:P:12:LYS:HB3	20:A:43:C:H5''	1.99	0.45
2:C:6:HIS:O	2:C:10:PHE:N	2.49	0.45
5:F:35:ALA:HB2	5:F:67:MET:HB3	1.98	0.45
20:A:964:A:O5'	20:A:964:A:H8	1.99	0.45
1:B:108:ILE:HA	1:B:111:ARG:HG3	1.98	0.45
20:A:1392:G:O2'	20:A:1502:A:OP1	2.32	0.45
8:I:3:GLN:NE2	20:A:1130:A:O2'	2.42	0.45
20:A:1255:G:H1	20:A:1282:C:H42	1.64	0.45
20:A:367:U:OP1	23:Y:340:TYR:OH	2.30	0.45
15:P:81:ARG:HA	20:A:458(E):A:O2'	2.16	0.45
1:B:95:GLN:HB3	1:B:96:ARG:HD2	1.97	0.45
20:A:881:G:H2'	20:A:882:C:C6	2.51	0.45
23:Y:545:GLY:HA3	23:Y:583:LYS:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1533:C:H3'	20:A:1534:A:O4'	2.16	0.45
5:F:19:LEU:HD11	5:F:59:TYR:OH	2.16	0.45
23:Y:458:HIS:O	23:Y:462:ILE:HG12	2.17	0.45
20:A:1386:G:H2'	20:A:1387:G:H8	1.81	0.45
4:E:127:ASN:HD22	20:A:19:C:P	2.40	0.45
9:J:63:PHE:HD1	13:N:58:LYS:HA	1.80	0.45
1:B:220:ASP:HA	1:B:223:ILE:HD12	1.99	0.45
20:A:33:A:H2'	20:A:34:C:H6	1.81	0.45
20:A:68(I):G:N2	20:A:68(R):C:H1'	2.32	0.45
1:B:175:ARG:NH2	20:A:1076:C:H5'	2.31	0.45
23:Y:30:GLU:HG2	23:Y:31:ARG:N	2.32	0.45
1:B:169:LYS:O	1:B:172:ILE:HG12	2.16	0.45
23:Y:33:LEU:HD22	23:Y:65:ILE:HG22	1.99	0.45
23:Y:604:PRO:HB2	23:Y:649:LEU:HD12	1.99	0.45
11:L:11:VAL:HG13	16:Q:29:HIS:HD2	1.81	0.45
4:E:115:VAL:HG12	4:E:116:THR:H	1.81	0.45
20:A:1204:A:H3'	20:A:1205:U:C6	2.52	0.45
3:D:29:PRO:O	3:D:30:LYS:HB3	2.17	0.45
23:Y:652:MET:O	23:Y:652:MET:HG3	2.15	0.45
10:K:30:VAL:HG22	10:K:43:SER:O	2.16	0.45
12:M:113:PRO:HB2	12:M:114:ARG:H	1.53	0.45
23:Y:333:GLY:H	23:Y:371:ALA:HB2	1.82	0.45
12:M:56:LEU:O	12:M:60:VAL:HG23	2.16	0.45
20:A:237:C:H2'	20:A:238:G:H8	1.76	0.45
20:A:1157:A:N6	20:A:1178:G:H1'	2.32	0.45
16:Q:38:ARG:HD3	20:A:280:C:O2	2.17	0.45
6:G:31:MET:HE1	20:A:1374:A:H1'	1.99	0.45
20:A:578:C:O2'	20:A:728:A:N3	2.43	0.45
4:E:51:VAL:O	4:E:55:VAL:HG23	2.16	0.45
20:A:66:G:N2	20:A:172:A:N3	2.64	0.45
20:A:930:C:H2'	20:A:931:C:C6	2.51	0.45
21:W:64:G:N1	21:W:65:U:C4	2.85	0.45
3:D:22:LYS:O	3:D:26:CYS:HB3	2.17	0.45
1:B:155:LEU:HD11	1:B:159:PRO:HG3	1.98	0.45
14:O:8:LYS:O	14:O:12:ILE:HG13	2.16	0.45
16:Q:68:ARG:NH1	20:A:277:C:H5'	2.31	0.45
4:E:18:ARG:HA	20:A:15:G:H21	1.82	0.45
7:H:83:ILE:HA	7:H:136:GLU:O	2.16	0.45
16:Q:98:LEU:HD13	20:A:279:A:C5	2.51	0.45
20:A:566:G:H4'	20:A:567:G:H5'	1.99	0.45
20:A:415:A:H2'	20:A:416:G:C8	2.51	0.45
20:A:1352:C:H2'	20:A:1353:G:C8	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:Q:22:LEU:HD11	16:Q:39:SER:HB2	1.98	0.45
1:B:124:SER:O	1:B:126:GLU:N	2.44	0.45
12:M:15:VAL:HG12	12:M:45:VAL:HA	1.98	0.45
1:B:70:PHE:HD2	1:B:81:VAL:HB	1.81	0.45
9:J:51:ARG:HG2	9:J:59:SER:C	2.36	0.45
13:N:17:LYS:HG3	13:N:18:VAL:N	2.32	0.45
23:Y:538:TYR:HB3	23:Y:542:VAL:HB	1.99	0.45
23:Y:21:ILE:O	23:Y:23:ALA:N	2.50	0.45
5:F:63:TYR:CD2	5:F:63:TYR:N	2.84	0.45
20:A:699:C:H2'	20:A:700:G:H5'	1.98	0.45
15:P:68:ASP:O	15:P:71:ARG:HB3	2.17	0.45
11:L:108:ALA:C	11:L:121:GLY:HA3	2.37	0.45
2:C:30:ARG:O	2:C:34:LEU:HG	2.17	0.45
21:W:20:U:H4'	21:W:20(A):U:C6	2.52	0.45
3:D:122:ARG:HD3	3:D:136:PRO:HD3	1.99	0.45
20:A:553:A:H2'	20:A:554:C:C6	2.52	0.45
23:Y:315:LYS:HD3	23:Y:316:ILE:N	2.31	0.45
20:A:1015:A:H1'	20:A:1218:C:O2'	2.17	0.45
23:Y:213:HIS:O	23:Y:216:LEU:HB3	2.17	0.45
23:Y:519:ARG:NH2	23:Y:678:GLU:H	2.15	0.45
20:A:834:C:H2'	20:A:835:U:H6	1.82	0.45
20:A:490:G:H2'	20:A:491:G:C8	2.51	0.45
23:Y:137:ASN:ND2	23:Y:263:ALA:N	2.56	0.45
1:B:171:ALA:HA	1:B:174:VAL:H	1.82	0.45
20:A:519:C:N4	20:A:520:A:C6	2.84	0.45
20:A:860:A:H2'	20:A:861:G:O4'	2.17	0.45
18:S:49:ILE:HD12	18:S:60:VAL:HG13	1.99	0.45
20:A:226:G:H2'	20:A:227:G:H8	1.81	0.45
20:A:1253:G:H1'	20:A:1355:G:O2'	2.17	0.45
4:E:70:PRO:HG2	4:E:142:LEU:HD22	1.98	0.45
1:B:141:GLU:O	1:B:145:LEU:HB2	2.16	0.45
2:C:43:LEU:HD22	2:C:47:LEU:HD22	1.98	0.45
20:A:691:G:H1'	20:A:696:A:H61	1.82	0.45
2:C:119:ARG:O	2:C:123:GLN:HG2	2.17	0.45
9:J:45:ARG:HG3	20:A:1254:C:OP1	2.17	0.45
19:T:38:LYS:HA	19:T:41:ILE:HG22	1.99	0.45
2:C:178:LEU:HD23	20:A:1112:C:H42	1.82	0.45
15:P:28:ARG:CZ	15:P:28:ARG:HB3	2.45	0.45
21:W:18:G:N2	21:W:58:A:O4'	2.50	0.45
20:A:961:U:H3	20:A:1201:A:H2	1.64	0.45
6:G:102:ARG:O	6:G:106:GLN:HG2	2.15	0.45
20:A:1102:A:H2'	20:A:1103:C:C6	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:534:ILE:HG13	23:Y:570:GLY:HA3	1.99	0.45
11:L:10:LEU:HB3	16:Q:32:TYR:CZ	2.52	0.45
2:C:49:SER:OG	2:C:83:ARG:NH2	2.42	0.45
20:A:151:A:H62	20:A:170:U:H3	1.64	0.45
4:E:36:ASP:OD1	4:E:40:ARG:N	2.50	0.45
20:A:195:A:N3	20:A:222:U:O2'	2.44	0.45
2:C:174:PRO:HA	20:A:1108:G:P	2.57	0.45
23:Y:416:LYS:HG2	23:Y:417:THR:HG23	1.98	0.45
20:A:1424:C:H2'	20:A:1425:U:O4'	2.17	0.45
5:F:18:GLN:O	5:F:21:LEU:HB3	2.17	0.45
14:O:41:GLU:HA	14:O:44:LYS:HG3	1.98	0.45
13:N:34:TYR:N	13:N:39:LEU:O	2.50	0.45
23:Y:24:GLY:O	26:Y:702:GDP:O2A	2.35	0.44
23:Y:22:ASP:O	26:Y:702:GDP:O3B	2.35	0.44
20:A:32:A:H1'	20:A:48:C:H41	1.82	0.44
20:A:551:U:H2'	20:A:552:U:C6	2.52	0.44
20:A:1317:C:H3'	20:A:1318:A:H8	1.82	0.44
25:Y:701:FUA:H322	25:Y:701:FUA:H16	1.75	0.44
1:B:179:LYS:NZ	20:A:1075:C:H5''	2.31	0.44
6:G:30:ILE:HD13	6:G:43:PHE:HB2	1.98	0.44
11:L:15:ARG:O	20:A:562:C:O2'	2.34	0.44
12:M:5:ALA:O	12:M:7:VAL:N	2.50	0.44
5:F:63:TYR:N	5:F:63:TYR:HD2	2.15	0.44
20:A:152:A:H3'	20:A:153:C:C6	2.52	0.44
4:E:29:GLY:HA2	4:E:46:GLY:O	2.17	0.44
20:A:198:G:H1	20:A:219:C:H42	1.65	0.44
20:A:838(A):U:O2'	20:A:838(B):C:H5''	2.16	0.44
3:D:105:VAL:HG21	3:D:126:ILE:HG13	1.99	0.44
20:A:1134:G:H2'	20:A:1135:U:O4'	2.18	0.44
20:A:1135:U:H2'	20:A:1137:C:O4'	2.17	0.44
23:Y:91:THR:HG22	23:Y:95:GLU:HG2	1.99	0.44
20:A:67:C:H2'	20:A:68:G:H8	1.77	0.44
23:Y:27:THR:HA	23:Y:30:GLU:HB3	1.99	0.44
4:E:78:HIS:O	4:E:93:PRO:HD3	2.18	0.44
5:F:46:ARG:NH2	17:R:37:VAL:HG21	2.32	0.44
20:A:757:U:H1'	20:A:879:C:H1'	1.99	0.44
23:Y:547:GLU:O	23:Y:551:GLN:NE2	2.48	0.44
20:A:794:A:H4'	20:A:1521:G:O2'	2.17	0.44
20:A:1170:A:O5'	20:A:1170:A:H8	2.00	0.44
3:D:105:VAL:HG21	3:D:121:VAL:HG22	1.98	0.44
5:F:84:ASN:O	5:F:86:ARG:N	2.48	0.44
20:A:1260:C:N4	20:A:1274:G:H1	2.15	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1285:A:H5'	20:A:1286:A:C8	2.51	0.44
23:Y:604:PRO:HA	23:Y:676:TYR:HB3	1.99	0.44
20:A:881:G:H2'	20:A:882:C:H6	1.81	0.44
7:H:103:VAL:HG11	7:H:109:ILE:H	1.81	0.44
20:A:582:U:H2'	20:A:583:A:C8	2.52	0.44
11:L:15:ARG:NH1	20:A:563:A:N3	2.65	0.44
15:P:19:ILE:HB	15:P:37:GLY:C	2.38	0.44
20:A:691:G:H1'	20:A:696:A:N6	2.32	0.44
23:Y:147:TRP:O	23:Y:151:ARG:HB2	2.17	0.44
17:R:19:LYS:HB3	17:R:20:ALA:H	1.61	0.44
20:A:1152:A:H2'	20:A:1153:C:H6	1.81	0.44
20:A:447:G:H2'	20:A:485:G:N2	2.31	0.44
18:S:15:LEU:HD23	18:S:15:LEU:HA	1.75	0.44
6:G:75:VAL:HG22	6:G:88:PRO:HB3	2.00	0.44
20:A:26:A:N6	20:A:558:G:H1'	2.32	0.44
20:A:32:A:H1'	20:A:48:C:N4	2.32	0.44
9:J:16:LEU:O	9:J:19:SER:OG	2.30	0.44
6:G:102:ARG:HD3	20:A:940:C:OP1	2.18	0.44
8:I:48:GLU:N	8:I:49:PRO:HD2	2.33	0.44
20:A:149:A:H2'	20:A:150:C:H6	1.83	0.44
23:Y:437:THR:OG1	23:Y:438:PHE:N	2.50	0.44
16:Q:46:ASP:OD2	16:Q:50:LYS:HG2	2.17	0.44
23:Y:344:THR:OG1	23:Y:390:VAL:HG13	2.17	0.44
6:G:78:ARG:HD3	6:G:154:TYR:O	2.18	0.44
11:L:33:ARG:N	11:L:85:ILE:HB	2.33	0.44
23:Y:201:ILE:HG12	23:Y:206:LEU:N	2.25	0.44
20:A:35:G:H2'	20:A:36:C:C6	2.53	0.44
16:Q:10:VAL:HG21	16:Q:51:TYR:HB3	1.99	0.44
6:G:102:ARG:NH2	20:A:939:G:H5''	2.32	0.44
22:V:6:G:H2'	22:V:7:G:C8	2.53	0.44
5:F:100:ASN:ND2	17:R:23:LYS:HG2	2.32	0.44
8:I:10:ARG:HG2	8:I:105:ASP:HB2	1.98	0.44
7:H:25:ASP:OD2	7:H:26:VAL:N	2.50	0.44
20:A:1403:C:H1'	20:A:1500:A:N1	2.32	0.44
6:G:91:VAL:HB	6:G:96:GLN:HG3	2.00	0.44
20:A:1326:C:H2'	20:A:1327:C:C6	2.53	0.44
3:D:12:CYS:SG	3:D:21:LEU:HD12	2.58	0.44
1:B:20:GLU:HG3	1:B:191:ASP:N	2.32	0.44
1:B:57:PHE:CD2	1:B:185:ILE:HD11	2.53	0.44
11:L:95:GLY:O	11:L:97:ARG:N	2.50	0.44
20:A:130:A:N1	20:A:233:C:H1'	2.32	0.44
16:Q:69:LYS:CG	20:A:254:G:H5''	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:15:GLU:OE2	3:D:63:LYS:HG3	2.17	0.44
20:A:68:G:H2'	20:A:68(A):G:O4'	2.18	0.44
16:Q:62:SER:HB2	16:Q:72:ARG:HG3	1.99	0.44
20:A:1181:G:O2'	20:A:1182:G:N7	2.50	0.44
20:A:226:G:H2'	20:A:227:G:C8	2.53	0.44
15:P:18:ARG:HD3	15:P:35:LYS:HD2	2.00	0.44
20:A:329:A:C5	20:A:332:G:C6	3.06	0.44
10:K:44:SER:OG	10:K:45:GLY:N	2.48	0.44
16:Q:7:THR:HA	16:Q:58:GLU:HA	1.99	0.44
3:D:200:GLU:O	3:D:204:ILE:HG12	2.18	0.44
11:L:73:GLU:HA	20:A:521:G:OP1	2.17	0.44
23:Y:18:ALA:HA	23:Y:25:LYS:HD3	2.00	0.44
20:A:1513:A:H2'	20:A:1514:C:H6	1.83	0.44
20:A:1149:C:H2'	20:A:1150:U:C6	2.53	0.44
20:A:672:U:O2'	20:A:673:G:O5'	2.27	0.44
9:J:16:LEU:HD21	9:J:70:ARG:HD3	2.00	0.44
20:A:501:C:H2'	20:A:502:G:H8	1.82	0.44
11:L:114:LYS:HA	11:L:117:ARG:HH11	1.83	0.44
18:S:78:ARG:HH11	20:A:1225:A:H5'	1.82	0.44
23:Y:118:SER:C	23:Y:120:THR:H	2.21	0.44
20:A:62:U:H5''	20:A:385:C:H1'	1.99	0.44
23:Y:103:GLY:HA2	23:Y:130:VAL:HG23	1.99	0.44
12:M:111:LYS:HB3	12:M:111:LYS:HE2	1.69	0.44
20:A:123:C:OP1	20:A:311:C:O2'	2.33	0.44
1:B:158:LEU:HA	1:B:159:PRO:HD3	1.78	0.44
1:B:187:LEU:HB2	1:B:201:ILE:HB	1.99	0.44
20:A:48:C:H2'	20:A:365:U:O4	2.18	0.44
16:Q:70:ARG:HH22	20:A:234:C:H5''	1.83	0.44
10:K:114:VAL:O	20:A:675:A:O2'	2.26	0.44
12:M:104:ARG:HA	20:A:1226:C:C4	2.53	0.44
8:I:89:ASN:HB3	8:I:92:TYR:HD1	1.82	0.44
4:E:35:GLY:N	4:E:112:LEU:HD13	2.33	0.44
23:Y:663:THR:C	23:Y:665:GLY:H	2.21	0.44
20:A:1352:C:H2'	20:A:1353:G:H8	1.82	0.44
20:A:198:G:H2'	20:A:199:G:H8	1.82	0.44
20:A:1170:A:C5	20:A:1171:G:H1'	2.52	0.44
23:Y:165:GLN:HB3	23:Y:177:ILE:HG21	2.00	0.44
15:P:33:ILE:HD13	20:A:229:U:H5''	1.99	0.44
1:B:32:ILE:HA	1:B:32:ILE:HD13	1.79	0.44
21:W:64:G:C2	21:W:65:U:N3	2.85	0.44
23:Y:497:PHE:HD2	23:Y:507:TYR:HA	1.82	0.44
20:A:677:U:H3	20:A:713:G:H22	1.64	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1127:G:H2'	20:A:1128:C:O4'	2.18	0.44
11:L:30:ALA:HA	20:A:363:A:N6	2.33	0.44
3:D:60:GLU:O	3:D:63:LYS:HB3	2.16	0.44
23:Y:311:ALA:HB3	23:Y:389:LEU:O	2.18	0.44
20:A:54:C:O2'	20:A:55:A:H5'	2.18	0.44
11:L:5:PRO:HB2	11:L:10:LEU:HG	1.99	0.44
4:E:118:ILE:HG13	4:E:120:THR:HG22	1.99	0.44
5:F:9:VAL:HB	5:F:87:ARG:CB	2.48	0.44
23:Y:406:GLU:HG3	23:Y:407:PRO:HD2	1.99	0.44
3:D:96:LEU:HD12	3:D:139:ARG:HH22	1.83	0.44
12:M:54:VAL:O	12:M:57:ARG:HG2	2.18	0.44
2:C:5:ILE:HD11	13:N:58:LYS:HE3	2.00	0.43
13:N:27:CYS:CB	20:A:1202:G:H21	2.30	0.43
11:L:97:ARG:HG2	11:L:97:ARG:H	1.53	0.43
1:B:194:PRO:O	1:B:196:LEU:N	2.51	0.43
20:A:1420:C:N4	20:A:1480:G:H1	2.16	0.43
14:O:7:GLU:O	14:O:11:VAL:HG23	2.18	0.43
6:G:26:PHE:CD2	6:G:30:ILE:HD11	2.53	0.43
23:Y:7:TYR:CE2	23:Y:9:LEU:HG	2.53	0.43
4:E:110:LEU:HB3	4:E:115:VAL:CG2	2.48	0.43
4:E:115:VAL:HG12	4:E:116:THR:N	2.33	0.43
1:B:22:LYS:HA	1:B:24:TRP:HD1	1.83	0.43
20:A:1343:G:H2'	20:A:1344:C:H6	1.82	0.43
2:C:182:ILE:HG12	2:C:203:PHE:HA	1.99	0.43
20:A:1107:C:C4	20:A:1108:G:C8	3.05	0.43
1:B:217:ARG:O	1:B:221:LEU:HB2	2.18	0.43
4:E:7:GLU:O	4:E:34:VAL:HA	2.18	0.43
23:Y:160:ARG:HH22	23:Y:222:ASP:HB2	1.83	0.43
20:A:1476:G:H2'	20:A:1477:C:C6	2.52	0.43
10:K:97:ALA:O	10:K:101:SER:OG	2.18	0.43
12:M:75:ALA:O	12:M:79:LYS:HG3	2.18	0.43
23:Y:133:ILE:HD13	23:Y:133:ILE:H	1.83	0.43
23:Y:607:ARG:HG2	23:Y:646:PHE:CE1	2.52	0.43
9:J:51:ARG:HB3	20:A:1060:C:C4'	2.46	0.43
13:N:6:LEU:HB3	13:N:23:ARG:NH2	2.33	0.43
2:C:157:ILE:HB	2:C:164:ARG:HH21	1.83	0.43
20:A:1304:G:H1'	20:A:1333:A:H61	1.83	0.43
20:A:68(C):C:H2'	20:A:68(D):C:C6	2.54	0.43
21:W:28:A:H2	21:W:42:U:H3	1.62	0.43
20:A:971:G:H3'	20:A:971:G:OP1	2.18	0.43
4:E:101:ILE:HG13	4:E:118:ILE:O	2.18	0.43
20:A:161:A:H61	20:A:347:G:HO2'	1.61	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:124:GLY:O	3:D:132:ARG:HB2	2.18	0.43
13:N:8:GLU:HA	13:N:11:LYS:HB2	1.99	0.43
20:A:303:A:H2'	20:A:304:U:O4'	2.18	0.43
23:Y:259:PHE:CB	23:Y:272:LEU:HD13	2.48	0.43
10:K:30:VAL:O	10:K:42:TRP:HA	2.18	0.43
11:L:78:GLN:HG3	11:L:79:GLU:H	1.82	0.43
23:Y:425:SER:HA	23:Y:428:LEU:HD23	2.00	0.43
8:I:118:LYS:HD2	20:A:1349:A:OP2	2.18	0.43
4:E:20:GLN:N	4:E:23:GLY:O	2.51	0.43
20:A:947:G:H4'	20:A:1332:A:H2	1.83	0.43
20:A:784:C:H2'	20:A:785:G:H8	1.83	0.43
20:A:68(K):U:H2'	20:A:68(M):U:C5	2.53	0.43
23:Y:496:LYS:HG3	23:Y:509:HIS:CG	2.53	0.43
23:Y:28:THR:HG21	23:Y:107:VAL:HG21	2.00	0.43
23:Y:28:THR:O	23:Y:32:ILE:HG12	2.18	0.43
20:A:1346:A:N1	20:A:1374:A:H5"	2.32	0.43
2:C:156:ARG:HE	2:C:159:GLY:HA2	1.83	0.43
20:A:833:U:O2'	20:A:834:C:O5'	2.30	0.43
23:Y:188:TYR:OH	23:Y:270:GLN:HG2	2.18	0.43
20:A:118:U:O4	20:A:288:A:H2'	2.18	0.43
2:C:114:PRO:HA	2:C:185:GLY:HA3	1.99	0.43
20:A:134:A:H2'	20:A:135:C:C6	2.54	0.43
20:A:919:A:O5'	20:A:919:A:H8	2.02	0.43
3:D:61:LYS:HE2	3:D:206:PHE:CE2	2.53	0.43
3:D:57:ARG:HG3	3:D:206:PHE:HB2	2.00	0.43
23:Y:491:VAL:O	23:Y:514:VAL:HG22	2.18	0.43
20:A:719:C:H2'	20:A:720:C:O4'	2.18	0.43
20:A:1317:C:H3'	20:A:1318:A:C8	2.54	0.43
20:A:130:A:H2	20:A:263:A:C2	2.37	0.43
23:Y:322:VAL:HG23	23:Y:325:LEU:HD11	1.99	0.43
2:C:4:LYS:HE3	20:A:1191:A:C5'	2.45	0.43
20:A:987:G:H1	20:A:1218:C:H42	1.65	0.43
4:E:42:GLY:HA3	4:E:62:ALA:O	2.18	0.43
7:H:13:ILE:O	7:H:17:THR:HG23	2.19	0.43
16:Q:82:MET:O	16:Q:86:GLU:HB2	2.18	0.43
20:A:563:A:O4'	20:A:566:G:N2	2.51	0.43
8:I:70:LYS:O	8:I:74:ILE:HG13	2.18	0.43
23:Y:555:LEU:HB2	23:Y:556:ILE:HD13	2.00	0.43
1:B:213:LEU:O	1:B:217:ARG:HB2	2.19	0.43
15:P:16:HIS:HE1	15:P:38:TYR:HB2	1.82	0.43
7:H:78:GLN:HE21	7:H:80:ILE:HB	1.82	0.43
15:P:40:ASP:HA	15:P:41:PRO:HD2	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:R:68:LYS:HB3	17:R:72:ARG:NH2	2.33	0.43
20:A:1489:G:H2'	20:A:1490:C:O4'	2.19	0.43
11:L:33:ARG:H	11:L:85:ILE:HB	1.83	0.43
1:B:101:MET:HB3	1:B:152:PHE:CE1	2.52	0.43
1:B:186:ALA:O	1:B:201:ILE:HG12	2.19	0.43
20:A:1307:U:H2'	20:A:1308:U:O4'	2.19	0.43
18:S:39:THR:HB	18:S:41:VAL:HG13	2.00	0.43
18:S:40:ILE:HG12	18:S:71:LEU:HA	2.00	0.43
20:A:1401:G:H5''	22:V:22:A:H61	1.83	0.43
20:A:1533:C:N4	22:V:12:A:N1	2.67	0.43
23:Y:543:GLN:O	23:Y:546:ILE:HB	2.19	0.43
20:A:834:C:H2'	20:A:835:U:C6	2.53	0.43
20:A:680:C:H2'	20:A:681:C:C6	2.53	0.43
20:A:1066:C:H3'	20:A:1067:A:C8	2.53	0.43
11:L:82:VAL:O	11:L:104:VAL:HG11	2.18	0.43
10:K:113:PRO:CB	20:A:676:A:H5''	2.46	0.43
20:A:68(G):G:C5	20:A:68(H):G:H1'	2.53	0.43
20:A:68(H):G:H2'	20:A:68(I):G:C8	2.54	0.43
19:T:52:ALA:HA	19:T:55:ILE:HB	2.00	0.43
21:W:27:C:H2'	21:W:28:A:H8	1.84	0.43
23:Y:627:ARG:O	23:Y:629:GLY:N	2.52	0.43
23:Y:188:TYR:CD2	23:Y:188:TYR:N	2.87	0.43
1:B:140:HIS:O	1:B:144:ARG:HG2	2.18	0.43
20:A:922:G:H2'	20:A:923:A:C8	2.53	0.43
1:B:161:ALA:HA	1:B:183:PRO:HB2	1.99	0.43
14:O:32:LEU:HA	14:O:35:ARG:HD2	2.00	0.43
3:D:138:TYR:HB2	20:A:620:C:H1'	2.01	0.43
10:K:38:ASN:HA	10:K:39:PRO:HD3	1.74	0.43
16:Q:25:ARG:NH1	20:A:237:C:H5''	2.32	0.43
20:A:1219:U:H2'	20:A:1220:G:C8	2.53	0.43
20:A:583:A:N6	20:A:758:G:O2'	2.51	0.43
20:A:389:A:C6	20:A:390:C:H1'	2.54	0.43
3:D:49:ARG:HB3	3:D:50:ARG:H	1.58	0.43
3:D:106:TYR:HB2	3:D:117:ALA:HB2	2.01	0.43
23:Y:190:ASN:HD21	23:Y:195:ASP:H	1.67	0.43
10:K:65:ALA:HB1	10:K:98:LEU:HD23	2.00	0.43
9:J:15:THR:HA	9:J:18:ALA:HB3	2.00	0.43
1:B:208:ILE:HD12	1:B:208:ILE:H	1.84	0.43
14:O:46:HIS:O	14:O:48:LYS:N	2.52	0.43
11:L:102:ARG:HA	11:L:107:ALA:HB3	2.01	0.43
20:A:956:U:H2'	20:A:957:U:O4'	2.19	0.43
18:S:10:PHE:CD2	20:A:1318:A:H4'	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:92:TYR:O	8:I:96:LEU:HB2	2.19	0.43
1:B:12:GLU:C	1:B:14:GLY:H	2.21	0.43
15:P:72:ARG:NH1	20:A:452:A:N3	2.66	0.43
2:C:176:HIS:HB2	20:A:1108:G:P	2.59	0.43
12:M:23:TYR:CZ	20:A:1330:U:H4'	2.54	0.43
12:M:88:ARG:HA	12:M:98:VAL:HG13	2.00	0.43
2:C:113:ALA:HB2	2:C:202:ILE:HG13	2.01	0.43
20:A:514:C:H2'	20:A:515:G:O4'	2.19	0.43
3:D:100:ARG:O	3:D:104:VAL:HG23	2.18	0.43
5:F:5:GLU:HB3	5:F:62:TRP:CZ2	2.53	0.43
20:A:955:U:H2'	20:A:956:U:O4'	2.19	0.43
20:A:1229:A:H5''	21:W:29:U:O2'	2.17	0.43
1:B:42:ILE:HG23	1:B:44:LEU:HG	2.01	0.43
5:F:21:LEU:O	5:F:25:ILE:HG12	2.19	0.43
20:A:637:G:H2'	20:A:638:G:O4'	2.19	0.43
11:L:58:VAL:HG11	11:L:85:ILE:CG1	2.46	0.43
20:A:33:A:H5''	20:A:364:A:H1'	2.01	0.43
11:L:30:ALA:HA	11:L:31:PRO:HD3	1.72	0.43
20:A:68(A):G:C2	20:A:68(B):G:C8	3.07	0.43
20:A:867:G:H2'	20:A:868:C:C6	2.54	0.43
19:T:89:ARG:NH2	20:A:186(A):C:O3'	2.52	0.43
4:E:110:LEU:HD13	4:E:115:VAL:HG21	2.01	0.43
20:A:479:C:H2'	20:A:480:U:C6	2.54	0.43
7:H:31:PHE:O	7:H:35:ILE:HG12	2.19	0.43
20:A:1108:G:H2'	20:A:1109:C:H5'	2.01	0.43
20:A:62:U:H2'	20:A:63:C:H6	1.84	0.43
2:C:34:LEU:HD22	13:N:25:VAL:HG21	2.00	0.43
5:F:18:GLN:O	5:F:22:GLU:HG2	2.18	0.43
5:F:5:GLU:HB3	5:F:62:TRP:HZ2	1.83	0.43
20:A:1410:G:H2'	20:A:1411:C:C6	2.53	0.43
23:Y:357:ARG:NH1	23:Y:373:ASP:OD1	2.52	0.43
3:D:37:PRO:O	3:D:38:TYR:HB3	2.19	0.43
20:A:301:G:H2'	20:A:302:G:C8	2.53	0.42
23:Y:201:ILE:C	23:Y:203:GLU:H	2.22	0.42
2:C:102:ASN:ND2	2:C:104:GLN:HG2	2.28	0.42
20:A:957:U:H1'	20:A:960:U:N3	2.33	0.42
12:M:115:LYS:H	20:A:1228:C:H5'	1.84	0.42
16:Q:63:ARG:HB2	20:A:130:A:C8	2.54	0.42
12:M:105:THR:HG22	20:A:1229:A:H61	1.85	0.42
15:P:80:PHE:O	20:A:458(E):A:H4'	2.18	0.42
1:B:95:GLN:HG3	1:B:147:LYS:HG3	2.01	0.42
23:Y:328:ILE:HG13	23:Y:330:VAL:H	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:M:77:ASN:O	12:M:81:LEU:HD13	2.19	0.42
2:C:36:ASP:OD1	2:C:57:ILE:HD13	2.19	0.42
20:A:62:U:OP1	20:A:385:C:O2'	2.35	0.42
20:A:197:A:N3	20:A:198:G:H1'	2.34	0.42
20:A:1210:C:H1'	20:A:1214:C:O2	2.18	0.42
20:A:1073:U:H2'	20:A:1074:G:H8	1.84	0.42
15:P:42:ARG:NH1	20:A:449:C:O2	2.52	0.42
20:A:358:U:OP1	23:Y:381:LYS:NZ	2.42	0.42
22:V:16:A:H2'	22:V:17:U:C6	2.54	0.42
8:I:28:VAL:N	8:I:31:GLN:O	2.48	0.42
7:H:115:SER:HB2	20:A:640:A:H1'	1.99	0.42
9:J:99:LYS:HA	9:J:99:LYS:HD2	1.68	0.42
19:T:36:LEU:HA	19:T:36:LEU:HD13	1.83	0.42
11:L:120:TYR:CD2	11:L:120:TYR:N	2.87	0.42
11:L:17:LYS:NZ	20:A:303:A:H5'	2.34	0.42
3:D:54:TYR:HA	3:D:57:ARG:HE	1.83	0.42
3:D:61:LYS:HD3	3:D:207:TYR:OH	2.20	0.42
20:A:909:A:H2'	20:A:910:C:O4'	2.19	0.42
20:A:756:C:O2'	20:A:878:G:N2	2.52	0.42
20:A:1148:U:H2'	20:A:1149:C:O4'	2.18	0.42
20:A:266:G:O2'	20:A:268:C:OP2	2.22	0.42
23:Y:603:GLU:HG2	23:Y:679:VAL:HG13	2.00	0.42
20:A:1313:U:H2'	20:A:1314:C:C6	2.54	0.42
1:B:12:GLU:HB3	1:B:44:LEU:HD22	2.01	0.42
20:A:745:C:H1'	20:A:836:G:O2'	2.19	0.42
20:A:487:A:H2'	20:A:488:C:O4'	2.19	0.42
22:V:18:G:H8	22:V:18:G:OP2	2.01	0.42
21:W:35:A:N6	22:V:18:G:O6	2.51	0.42
9:J:35:SER:N	9:J:73:ASP:O	2.46	0.42
23:Y:86:GLY:O	23:Y:88:VAL:N	2.52	0.42
3:D:24:GLU:O	3:D:28:SER:HB3	2.19	0.42
20:A:158:G:H2'	20:A:159:G:O4'	2.19	0.42
8:I:29:ASN:HB2	8:I:65:VAL:H	1.84	0.42
19:T:87:LYS:HA	19:T:87:LYS:HD2	1.84	0.42
5:F:90:VAL:O	20:A:736:C:O2'	2.18	0.42
20:A:431:A:H2'	20:A:432:A:C8	2.54	0.42
20:A:68(H):G:N2	20:A:68(R):C:C2	2.84	0.42
7:H:10:LEU:O	7:H:13:ILE:HB	2.19	0.42
6:G:115:ARG:O	6:G:119:ARG:HG3	2.20	0.42
23:Y:523:PHE:CE2	23:Y:547:GLU:HG2	2.54	0.42
20:A:1152:A:H2'	20:A:1153:C:C6	2.55	0.42
20:A:443:C:H2'	20:A:444:C:C6	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1366:C:H2'	20:A:1367:C:C6	2.55	0.42
20:A:386:C:H2'	20:A:387:U:O4'	2.20	0.42
20:A:652:U:H3	20:A:753:A:H62	1.66	0.42
20:A:113:G:H2'	20:A:114:U:C6	2.53	0.42
4:E:125:SER:C	4:E:127:ASN:H	2.23	0.42
11:L:69:TYR:CE1	11:L:70:ILE:HG13	2.54	0.42
1:B:219:VAL:O	1:B:223:ILE:HG13	2.19	0.42
13:N:29:ARG:HH22	20:A:974:A:P	2.42	0.42
17:R:71:LYS:HE2	20:A:719:C:N4	2.35	0.42
11:L:104:VAL:C	11:L:105:TYR:HD1	2.22	0.42
18:S:36:ARG:HD3	20:A:1221:G:H5'	2.01	0.42
20:A:68(B):G:H3'	20:A:68(C):C:H6	1.84	0.42
20:A:68(L):U:H5''	20:A:68(M):U:OP2	2.20	0.42
8:I:49:PRO:HD3	8:I:101:PHE:HE2	1.84	0.42
21:W:69:A:H2'	21:W:70:G:C8	2.49	0.42
20:A:778:G:H2'	20:A:779:C:O4'	2.19	0.42
20:A:163:C:H2'	20:A:164:U:C6	2.54	0.42
23:Y:519:ARG:HH12	23:Y:678:GLU:HB2	1.84	0.42
12:M:111:LYS:HG2	12:M:112:GLY:H	1.84	0.42
20:A:507:C:P	20:A:508:C:H3'	2.60	0.42
19:T:28:ALA:O	19:T:31:SER:OG	2.28	0.42
20:A:680:C:H2'	20:A:681:C:H6	1.84	0.42
1:B:69:LEU:HG	1:B:159:PRO:HG2	2.02	0.42
20:A:713:G:OP2	20:A:713:G:H8	2.02	0.42
10:K:109:VAL:HA	17:R:85:LEU:O	2.19	0.42
23:Y:255:ILE:HA	23:Y:255:ILE:HD12	1.74	0.42
23:Y:70:THR:HG23	23:Y:358:MET:SD	2.59	0.42
3:D:158:ILE:O	3:D:162:LEU:HG	2.20	0.42
20:A:339:C:H2'	20:A:340:U:H6	1.81	0.42
20:A:328:C:H4'	20:A:329:A:C5'	2.49	0.42
2:C:156:ARG:H	2:C:196:LEU:HD12	1.84	0.42
8:I:37:PHE:CD2	8:I:70:LYS:HG3	2.54	0.42
8:I:71:SER:HA	8:I:74:ILE:HG13	2.01	0.42
20:A:169:C:H2'	20:A:170:U:C6	2.54	0.42
20:A:695:A:H2'	20:A:696:A:C8	2.54	0.42
20:A:609:A:H2'	20:A:610:G:O4'	2.20	0.42
17:R:53:ARG:HD2	17:R:63:GLN:HE21	1.83	0.42
23:Y:398:ILE:HG22	23:Y:399:LEU:H	1.84	0.42
23:Y:25:LYS:CG	26:Y:702:GDP:O2B	2.68	0.42
3:D:22:LYS:HD3	20:A:409:G:OP2	2.19	0.42
8:I:5:TYR:HH	20:A:1147:C:HO2'	1.66	0.42
9:J:19:SER:O	9:J:23:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:57:GLU:H	6:G:57:GLU:CD	2.23	0.42
20:A:776:G:N2	20:A:803:G:N7	2.67	0.42
23:Y:614:GLU:CD	23:Y:614:GLU:H	2.22	0.42
23:Y:511:LYS:HB3	23:Y:568:TYR:CZ	2.54	0.42
21:W:27:C:H2'	21:W:28:A:C8	2.55	0.42
15:P:20:VAL:HG21	15:P:32:TYR:CD1	2.54	0.42
20:A:971:G:H22	20:A:1363:A:P	2.42	0.42
7:H:62:TYR:N	7:H:62:TYR:CD2	2.87	0.42
3:D:134:ASP:HB2	3:D:135:LEU:H	1.58	0.42
1:B:218:ALA:O	1:B:221:LEU:HB3	2.19	0.42
5:F:50:TYR:HA	5:F:51:PRO:HD2	1.77	0.42
23:Y:188:TYR:HD2	23:Y:188:TYR:N	2.17	0.42
6:G:137:LYS:HA	6:G:140:ASP:HB3	2.00	0.42
20:A:623:C:H2'	20:A:624:C:C6	2.55	0.42
12:M:84:ILE:HB	18:S:74:PHE:CE1	2.55	0.42
20:A:1195:C:H5''	20:A:1196:U:OP2	2.18	0.42
16:Q:53:LEU:HG	16:Q:53:LEU:H	1.66	0.42
8:I:4:TYR:HA	8:I:87:GLN:OE1	2.20	0.42
10:K:120:ARG:HH22	20:A:1525:G:P	2.42	0.42
9:J:54:PHE:CD1	9:J:55:LYS:HD2	2.55	0.42
2:C:150:LYS:O	2:C:201:TYR:HB2	2.20	0.42
8:I:11:LYS:HE3	20:A:1371:G:OP2	2.20	0.42
7:H:12:ARG:O	7:H:15:ASN:HB2	2.20	0.42
23:Y:537:GLU:HG3	23:Y:538:TYR:CD1	2.55	0.42
20:A:1340:A:C6	20:A:1341:U:C4	3.08	0.42
20:A:186(C):G:O6	20:A:186(N):U:O2	2.37	0.42
23:Y:519:ARG:NH1	23:Y:678:GLU:HB2	2.34	0.42
7:H:71:GLY:O	7:H:73:ASP:N	2.52	0.42
23:Y:83:ASP:O	23:Y:85:PRO:HD3	2.19	0.42
6:G:151:TYR:HA	6:G:154:TYR:CD1	2.55	0.42
1:B:69:LEU:N	1:B:163:PHE:H	2.15	0.42
20:A:1003:G:C2	20:A:1037:C:O2	2.73	0.42
8:I:5:TYR:HA	8:I:17:VAL:O	2.19	0.42
20:A:889:A:H4'	20:A:890:G:H4'	2.02	0.42
19:T:43:LEU:CB	19:T:52:ALA:HB2	2.48	0.42
23:Y:647:VAL:HA	23:Y:648:PRO:HD3	1.89	0.42
4:E:70:PRO:HG2	4:E:142:LEU:HD13	2.02	0.42
14:O:61:GLY:O	14:O:65:ARG:HG3	2.20	0.42
23:Y:443:HIS:ND1	23:Y:446:THR:HG22	2.35	0.42
20:A:371:G:H21	20:A:374:A:N6	2.18	0.42
20:A:1386:G:H2'	20:A:1387:G:C8	2.55	0.42
15:P:22:THR:HA	15:P:33:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:173:TRP:CH2	3:D:194:LEU:HD21	2.54	0.42
19:T:25:ARG:HB2	19:T:25:ARG:CZ	2.46	0.42
20:A:766:A:C8	20:A:814:A:N6	2.88	0.42
20:A:1126:U:H2'	20:A:1127:G:O4'	2.19	0.42
11:L:79:GLU:O	11:L:80:HIS:CG	2.72	0.42
20:A:978:A:C6	20:A:1318:A:C6	3.08	0.42
12:M:87:TYR:HA	12:M:90:LEU:HB3	2.02	0.42
23:Y:162:VAL:HB	23:Y:255:ILE:CG1	2.48	0.42
20:A:598:U:H2'	20:A:599:C:H6	1.84	0.42
2:C:189:ALA:HB1	2:C:196:LEU:HD23	2.01	0.42
2:C:36:ASP:HA	2:C:39:ILE:HD12	2.00	0.42
23:Y:379:GLY:HA2	23:Y:381:LYS:HE3	2.00	0.42
20:A:443:C:H2'	20:A:444:C:H6	1.85	0.42
23:Y:414:GLU:HA	23:Y:415:PRO:HD2	1.86	0.42
7:H:20:TYR:OH	7:H:76:PRO:O	2.24	0.42
20:A:511:C:C2	20:A:512:U:C5	3.08	0.42
23:Y:474:ALA:O	23:Y:476:VAL:N	2.53	0.42
23:Y:212:TYR:O	23:Y:215:LYS:HB2	2.20	0.42
4:E:121:LYS:HD2	4:E:121:LYS:HA	1.73	0.42
1:B:69:LEU:HA	1:B:69:LEU:HD22	1.81	0.42
23:Y:201:ILE:HG22	23:Y:203:GLU:H	1.85	0.42
23:Y:608:VAL:HG13	23:Y:669:PHE:HB2	2.01	0.42
3:D:172:PRO:HB2	3:D:187:ARG:NH2	2.32	0.42
20:A:267:C:H2'	20:A:268:C:C6	2.55	0.42
23:Y:494:GLU:CG	23:Y:496:LYS:HB2	2.50	0.42
23:Y:271:LEU:H	23:Y:271:LEU:HG	1.69	0.42
7:H:10:LEU:HD22	7:H:83:ILE:HD11	2.02	0.42
1:B:209:ARG:HH11	1:B:239:VAL:HG13	1.84	0.42
20:A:829:G:H8	20:A:829:G:OP2	2.03	0.42
23:Y:179:ASP:OD1	23:Y:181:LEU:HB3	2.20	0.42
20:A:660:G:H2'	20:A:661:G:H8	1.85	0.42
3:D:96:LEU:HD12	3:D:139:ARG:NH2	2.35	0.42
20:A:420:U:N3	20:A:422:C:N3	2.68	0.42
10:K:69:ALA:HA	10:K:103:LEU:HD21	2.02	0.42
17:R:61:LYS:HE3	17:R:61:LYS:HB2	1.82	0.42
21:W:14:A:C2	21:W:22:G:H1'	2.54	0.41
23:Y:201:ILE:HG21	23:Y:206:LEU:N	2.35	0.41
11:L:92:ASP:CG	20:A:523:A:H61	2.16	0.41
20:A:1504:G:O2'	20:A:1505:G:O5'	2.36	0.41
9:J:55:LYS:HG3	20:A:973:G:C1'	2.50	0.41
12:M:120:LYS:NZ	20:A:955:U:H4'	2.35	0.41
25:Y:701:FUA:C20	25:Y:701:FUA:O1	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:W:38:A:H2'	21:W:39:U:O4'	2.20	0.41
20:A:22:G:H4'	20:A:885:G:C8	2.55	0.41
23:Y:580:MET:HA	23:Y:583:LYS:HB3	2.02	0.41
7:H:29:SER:HA	20:A:590:C:P	2.60	0.41
16:Q:9:VAL:HG22	16:Q:56:VAL:HG22	2.01	0.41
20:A:578:C:H2'	20:A:579:G:H8	1.82	0.41
2:C:91:LEU:O	2:C:95:THR:N	2.52	0.41
20:A:515:G:H2'	20:A:516:U:C6	2.55	0.41
23:Y:10:LYS:HG2	23:Y:284:LEU:HD22	2.01	0.41
21:W:50:C:N4	21:W:64:G:N1	2.31	0.41
3:D:115:ARG:NH1	20:A:407:G:OP1	2.53	0.41
20:A:18:C:H2'	20:A:19:C:C6	2.55	0.41
23:Y:526:VAL:CG2	23:Y:566:THR:HG23	2.50	0.41
20:A:755:G:H2'	20:A:756:C:C6	2.55	0.41
20:A:33:A:H5''	20:A:364:A:O2'	2.20	0.41
23:Y:13:ARG:HD3	23:Y:79:ILE:HG12	2.01	0.41
18:S:10:PHE:CG	20:A:1318:A:H4'	2.55	0.41
20:A:1415:G:H2'	20:A:1416:G:O4'	2.20	0.41
25:Y:701:FUA:H203	25:Y:701:FUA:H151	1.86	0.41
20:A:784:C:H2'	20:A:785:G:C8	2.56	0.41
11:L:113:ARG:HH12	20:A:537:G:P	2.43	0.41
20:A:241:C:H2'	20:A:242:C:H6	1.85	0.41
20:A:320:C:H2'	20:A:321:A:C8	2.55	0.41
7:H:41:ARG:HB3	7:H:41:ARG:HE	1.73	0.41
7:H:91:ARG:NH2	20:A:564:C:O3'	2.53	0.41
4:E:64:ARG:O	4:E:66:MET:N	2.53	0.41
20:A:382:A:H2'	20:A:383:A:C8	2.54	0.41
8:I:9:ARG:HB3	8:I:104:ARG:NH1	2.34	0.41
23:Y:168:ILE:H	23:Y:174:PHE:HE1	1.68	0.41
8:I:81:ILE:HG22	8:I:85:LEU:HD11	2.02	0.41
8:I:81:ILE:O	8:I:85:LEU:HG	2.19	0.41
20:A:110:C:H2'	20:A:111:G:O4'	2.20	0.41
23:Y:25:LYS:CB	26:Y:702:GDP:O2B	2.68	0.41
23:Y:206:LEU:HB3	23:Y:207:ASP:H	1.64	0.41
11:L:50:SER:HB2	20:A:519:C:OP2	2.20	0.41
11:L:34:ARG:HG3	11:L:82:VAL:CG1	2.49	0.41
16:Q:64:PRO:HD2	20:A:130:A:N7	2.35	0.41
16:Q:66:SER:HA	20:A:265:G:O3'	2.20	0.41
4:E:144:THR:O	4:E:148:VAL:HG23	2.20	0.41
23:Y:339:SER:O	23:Y:351:ARG:HD2	2.20	0.41
20:A:1534:A:O5'	20:A:1534:A:H8	2.03	0.41
23:Y:197:ARG:NH2	23:Y:198:GLU:HG2	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:Q:12:SER:HA	16:Q:14:LYS:NZ	2.35	0.41
14:O:33:THR:O	14:O:36:ILE:HB	2.20	0.41
15:P:25:ARG:HH22	20:A:134:A:H61	1.68	0.41
20:A:510:A:H5'	20:A:511:C:OP2	2.20	0.41
3:D:170:VAL:HG21	3:D:176:LEU:HB2	2.01	0.41
11:L:72:GLY:HA3	20:A:522:C:OP1	2.21	0.41
6:G:136:LYS:HD2	6:G:136:LYS:HA	1.91	0.41
12:M:36:LYS:HA	12:M:36:LYS:HD3	1.84	0.41
6:G:87:VAL:HG11	6:G:155:ARG:HA	2.01	0.41
4:E:125:SER:OG	4:E:125:SER:O	2.39	0.41
1:B:68:ILE:CG2	1:B:163:PHE:HB2	2.51	0.41
20:A:955:U:H2'	20:A:956:U:C6	2.55	0.41
20:A:426:G:H2'	20:A:427:U:O4'	2.20	0.41
20:A:244:U:O4	20:A:893:C:N3	2.53	0.41
20:A:626:U:H2'	20:A:627:G:H8	1.86	0.41
20:A:55:A:H2'	20:A:56:U:O4'	2.20	0.41
8:I:111:ARG:HG3	20:A:1369:C:OP2	2.21	0.41
7:H:97:VAL:HG12	20:A:600:C:OP1	2.19	0.41
16:Q:29:HIS:O	16:Q:31:LEU:N	2.54	0.41
23:Y:20:HIS:HB3	23:Y:118:SER:CA	2.51	0.41
23:Y:166:LEU:HB2	23:Y:178:ILE:HG22	2.02	0.41
15:P:66:PRO:CG	15:P:71:ARG:HH22	2.33	0.41
20:A:633:G:H2'	20:A:634:C:C6	2.55	0.41
10:K:14:VAL:HB	10:K:15:ALA:H	1.64	0.41
12:M:21:TYR:HD2	12:M:21:TYR:HA	1.70	0.41
23:Y:489:LYS:HE3	23:Y:489:LYS:HB2	1.87	0.41
3:D:101:LEU:O	3:D:105:VAL:HG23	2.21	0.41
3:D:57:ARG:NH1	3:D:205:GLU:HB3	2.36	0.41
11:L:83:VAL:HG11	11:L:100:ILE:HD13	2.01	0.41
23:Y:668:SER:HB2	23:Y:669:PHE:CD1	2.56	0.41
1:B:87:ARG:NH2	1:B:233:SER:OG	2.54	0.41
23:Y:329:ARG:O	23:Y:329:ARG:HG3	2.19	0.41
20:A:505:G:N2	20:A:526:C:N3	2.62	0.41
8:I:23:ASN:O	8:I:57:GLY:HA2	2.21	0.41
23:Y:30:GLU:HG2	23:Y:31:ARG:HG2	2.01	0.41
19:T:89:ARG:NH2	20:A:186(A):C:O2'	2.53	0.41
20:A:509:A:H2	20:A:543:C:O2	2.04	0.41
20:A:68(O):A:H3'	20:A:68(P):C:O4'	2.19	0.41
20:A:600:C:H2'	20:A:601:C:C6	2.55	0.41
8:I:69:GLY:HA2	20:A:1249:C:O2	2.21	0.41
4:E:75:THR:OG1	4:E:76:ILE:O	2.37	0.41
20:A:1051:C:H2'	20:A:1052:U:H6	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:652:U:O4	20:A:753:A:N7	2.53	0.41
20:A:993:G:C5	20:A:1046:A:C2	3.08	0.41
4:E:82:VAL:HG11	4:E:138:ALA:HA	2.03	0.41
20:A:395:C:H2'	20:A:396:G:H8	1.85	0.41
1:B:114:ARG:O	1:B:118:LEU:HG	2.21	0.41
21:W:64:G:C2	21:W:65:U:C4	3.09	0.41
23:Y:651:GLU:O	23:Y:652:MET:HB3	2.20	0.41
20:A:32:A:H2'	20:A:33:A:H8	1.82	0.41
20:A:1324:A:C4'	20:A:1362:C:H4'	2.48	0.41
20:A:978:A:OP2	20:A:1362(A):C:N4	2.53	0.41
20:A:986:A:H2'	20:A:987:G:C8	2.56	0.41
4:E:78:HIS:HB2	7:H:104:ARG:HG3	2.02	0.41
9:J:46:ARG:HD2	13:N:61:TRP:HZ3	1.86	0.41
7:H:29:SER:HA	20:A:590:C:OP1	2.21	0.41
19:T:18:GLN:O	19:T:22:ARG:HG3	2.21	0.41
20:A:715:A:H1'	20:A:777:A:N1	2.36	0.41
20:A:1093:A:O2'	20:A:1095:U:OP1	2.26	0.41
7:H:112:LEU:HA	7:H:134:ILE:HG13	2.03	0.41
19:T:88:VAL:O	19:T:92:LEU:HG	2.20	0.41
16:Q:27:PHE:O	16:Q:36:ILE:HG12	2.21	0.41
1:B:135:GLN:HA	1:B:138:LEU:HG	2.02	0.41
20:A:820:U:H3'	20:A:821:G:H5'	2.02	0.41
20:A:1110:A:H2'	20:A:1111:A:O4'	2.20	0.41
21:W:53:G:N2	21:W:61:C:N3	2.57	0.41
1:B:57:PHE:O	1:B:60:ASP:HB2	2.21	0.41
8:I:5:TYR:O	8:I:84:ALA:HA	2.21	0.41
14:O:38:ARG:HA	14:O:38:ARG:HD3	1.57	0.41
18:S:58:VAL:HG21	18:S:75:ALA:CB	2.50	0.41
20:A:1537:U:H2'	20:A:1538:C:H6	1.86	0.41
20:A:458:C:H2'	20:A:458(A):G:O4'	2.21	0.41
20:A:971:G:N2	20:A:1363:A:OP2	2.48	0.41
23:Y:247:ARG:HB2	23:Y:279:TYR:CD1	2.54	0.41
8:I:46:ALA:HB2	8:I:74:ILE:HG22	2.02	0.41
23:Y:655:TYR:OH	23:Y:659:LEU:HD23	2.20	0.41
6:G:119:ARG:NH2	20:A:1240:U:OP1	2.53	0.41
6:G:4:ARG:HG2	20:A:932:C:OP1	2.21	0.41
6:G:149:ARG:O	6:G:149:ARG:HD3	2.21	0.41
20:A:123:C:H5''	20:A:311:C:O2'	2.20	0.41
1:B:68:ILE:HG23	1:B:163:PHE:N	2.36	0.41
1:B:71:VAL:CG2	1:B:164:VAL:HG22	2.50	0.41
23:Y:341:VAL:HB	23:Y:342:TYR:H	1.74	0.41
23:Y:35:TYR:CE1	23:Y:266:ASN:HB3	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:9:LEU:HD13	23:Y:303:PRO:HB2	2.02	0.41
20:A:1404:C:H2'	20:A:1405:G:C8	2.55	0.41
8:I:70:LYS:NZ	20:A:1248:A:O2'	2.52	0.41
23:Y:181:LEU:HG	23:Y:182:ARG:HG3	2.02	0.41
10:K:62:GLN:HG3	10:K:97:ALA:HB2	2.03	0.41
23:Y:188:TYR:HA	23:Y:196:ILE:HB	2.03	0.41
20:A:604:G:H1	20:A:634:C:H42	1.69	0.41
1:B:128:GLU:HB3	1:B:129:GLU:H	1.69	0.41
15:P:55:ARG:O	15:P:58:TYR:HB3	2.20	0.41
20:A:1276:G:H2'	20:A:1277:C:C6	2.56	0.41
9:J:38:ILE:HG12	9:J:71:LEU:HB3	2.03	0.41
11:L:32:PHE:HA	11:L:85:ILE:O	2.21	0.41
20:A:429:U:H1'	20:A:430:A:H5''	2.03	0.41
1:B:187:LEU:HD22	1:B:188:ALA:N	2.36	0.41
20:A:302:G:H21	20:A:556:C:H4'	1.86	0.41
11:L:104:VAL:HG12	11:L:105:TYR:CD1	2.56	0.41
20:A:129(A):G:C6	20:A:186(H):U:H4'	2.56	0.41
23:Y:341:VAL:HG23	23:Y:350:GLU:HB2	2.03	0.41
20:A:862:C:H1'	20:A:874:G:H4'	2.02	0.41
23:Y:617:MET:HA	23:Y:620:VAL:HG22	2.01	0.41
5:F:99:ALA:HB2	17:R:31:LEU:HD21	2.02	0.41
23:Y:354:ARG:HH12	23:Y:378:VAL:HG11	1.86	0.41
13:N:53:LEU:HA	13:N:54:PRO:HD3	1.59	0.41
12:M:73:GLU:O	12:M:77:ASN:ND2	2.38	0.41
3:D:64:LEU:HD23	3:D:203:VAL:HG21	2.03	0.41
20:A:588:G:H1	20:A:651:C:N4	2.18	0.41
7:H:12:ARG:HH11	7:H:26:VAL:HG23	1.85	0.41
20:A:322:C:H5	20:A:328:C:H5	1.69	0.41
11:L:11:VAL:HG22	16:Q:32:TYR:HB3	2.03	0.41
20:A:115:G:O2'	20:A:116:A:P	2.78	0.41
8:I:69:GLY:O	8:I:73:GLN:N	2.49	0.41
5:F:2:ARG:CZ	5:F:69:GLU:HB3	2.51	0.41
20:A:1534:A:H2'	20:A:1535:C:C6	2.55	0.41
2:C:29:TYR:HE2	13:N:37:PHE:CD2	2.38	0.41
2:C:40:ARG:O	2:C:44:GLU:HG3	2.21	0.41
6:G:115:ARG:HH12	6:G:117:ALA:HB3	1.85	0.41
12:M:67:GLU:HB2	12:M:71:ARG:HH21	1.85	0.41
3:D:92:VAL:O	3:D:96:LEU:HD13	2.21	0.41
3:D:100:ARG:HH11	3:D:137:SER:HA	1.86	0.41
20:A:377:G:H1	20:A:386:C:H42	1.68	0.41
20:A:1196:U:O2	20:A:1196:U:H2'	2.21	0.41
1:B:178:ARG:HH22	7:H:71:GLY:H	1.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:85:LEU:HG	8:I:85:LEU:H	1.65	0.41
2:C:177:THR:HG23	20:A:1111:A:H2	1.86	0.41
20:A:138:G:H2'	20:A:139:G:C8	2.56	0.41
20:A:997:U:H2'	20:A:998:G:O4'	2.21	0.41
15:P:36:ILE:HB	15:P:52:ASP:HB3	2.01	0.41
8:I:128:ARG:HD3	8:I:128:ARG:H	1.86	0.41
16:Q:52:LYS:HE3	16:Q:52:LYS:HB3	1.64	0.41
1:B:83:MET:HB2	1:B:234:PRO:HG3	2.03	0.41
2:C:64:VAL:HB	2:C:99:VAL:HA	2.02	0.41
14:O:43:LEU:HD21	14:O:53:HIS:HB2	2.02	0.41
20:A:1465:C:H2'	20:A:1466:C:C6	2.56	0.41
9:J:43:ARG:HD3	9:J:43:ARG:HA	1.70	0.41
23:Y:412:ALA:HB2	23:Y:479:PRO:HA	2.03	0.41
21:W:14:A:H2'	21:W:15:G:O4'	2.21	0.41
11:L:84:LEU:HD13	11:L:104:VAL:CG1	2.50	0.41
20:A:1350:A:H2'	20:A:1351:U:H6	1.86	0.41
20:A:263:A:O2'	20:A:264:U:O5'	2.35	0.41
16:Q:67:LYS:C	16:Q:69:LYS:H	2.24	0.41
20:A:357:G:OP1	20:A:367:U:H5''	2.21	0.41
8:I:99:LEU:HD12	8:I:101:PHE:CE1	2.55	0.41
12:M:40:ASN:HA	12:M:41:PRO:HD3	1.84	0.41
7:H:88:LYS:H	7:H:91:ARG:HB2	1.86	0.41
20:A:764:C:H2'	20:A:765:G:C8	2.55	0.41
20:A:615:C:H2'	20:A:616:G:O4'	2.20	0.41
20:A:603:U:H2'	20:A:604:G:C8	2.56	0.41
20:A:1212:U:H5'	20:A:1213:A:OP1	2.20	0.41
20:A:961:U:C2	20:A:1201:A:N1	2.87	0.40
1:B:108:ILE:HG21	1:B:152:PHE:CE1	2.56	0.40
20:A:976:G:N2	20:A:1362(A):C:OP2	2.23	0.40
10:K:89:ALA:O	10:K:91:ARG:N	2.54	0.40
2:C:184:TYR:HB2	2:C:201:TYR:CD2	2.57	0.40
20:A:599:C:N4	20:A:639:G:H1	2.13	0.40
11:L:86:ARG:HB3	11:L:99:HIS:H	1.86	0.40
4:E:52:PRO:O	4:E:56:GLN:HG2	2.20	0.40
4:E:48:ALA:HA	4:E:49:PRO:HD3	1.93	0.40
20:A:1372:U:H2'	20:A:1373:G:O4'	2.20	0.40
14:O:5:LYS:CD	14:O:5:LYS:H	2.33	0.40
4:E:64:ARG:NE	4:E:64:ARG:HA	2.37	0.40
1:B:110:GLN:HA	1:B:113:HIS:HB2	2.02	0.40
19:T:53:LEU:HD23	19:T:53:LEU:HA	1.90	0.40
19:T:84:LEU:O	19:T:88:VAL:HG23	2.21	0.40
18:S:50:ALA:HA	18:S:59:PRO:HA	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:430:ARG:HB2	23:Y:430:ARG:CZ	2.51	0.40
4:E:127:ASN:O	4:E:131:ILE:HG12	2.21	0.40
9:J:52:GLY:HA2	20:A:1059:C:O2'	2.21	0.40
9:J:49:VAL:HG22	9:J:50:ILE:N	2.37	0.40
2:C:66:VAL:O	2:C:102:ASN:N	2.54	0.40
20:A:892:A:H2'	20:A:893:C:H6	1.86	0.40
1:B:133:LYS:HD3	20:A:1158:C:H5''	2.03	0.40
8:I:111:ARG:HD2	13:N:61:TRP:HE1	1.86	0.40
2:C:32:LEU:HD23	2:C:59:ARG:HH21	1.85	0.40
11:L:10:LEU:HB3	16:Q:32:TYR:CE1	2.56	0.40
16:Q:8:GLY:O	16:Q:56:VAL:HA	2.22	0.40
20:A:120:A:C6	20:A:122:G:C2	3.08	0.40
23:Y:197:ARG:HH21	23:Y:198:GLU:HG2	1.86	0.40
17:R:44:LEU:HD21	17:R:50:ILE:HG12	2.03	0.40
20:A:180:U:H2'	20:A:181:G:H5'	2.03	0.40
15:P:15:PRO:HD2	15:P:42:ARG:NE	2.37	0.40
6:G:121:ALA:O	6:G:125:MET:HG2	2.22	0.40
20:A:306:G:O2'	20:A:307:C:H5'	2.20	0.40
11:L:55:VAL:HG12	11:L:67:THR:HG22	2.03	0.40
6:G:87:VAL:HG13	6:G:151:TYR:O	2.22	0.40
3:D:112:VAL:O	3:D:113:SER:HB2	2.21	0.40
14:O:42:HIS:HE1	14:O:46:HIS:HD2	1.69	0.40
1:B:71:VAL:CB	1:B:164:VAL:HG22	2.51	0.40
13:N:29:ARG:O	13:N:33:VAL:HG21	2.21	0.40
16:Q:64:PRO:HG3	20:A:234:C:H4'	2.03	0.40
20:A:427:U:H5''	20:A:542:G:OP1	2.21	0.40
23:Y:339:SER:C	23:Y:352:VAL:HG13	2.42	0.40
5:F:97:PHE:O	17:R:31:LEU:HB2	2.21	0.40
7:H:127:LEU:HA	7:H:127:LEU:HD13	1.91	0.40
12:M:81:LEU:HB3	12:M:89:GLY:HA3	2.02	0.40
12:M:31:LYS:HA	12:M:34:LEU:HB2	2.03	0.40
8:I:107:ARG:NE	20:A:1347:G:O4'	2.55	0.40
16:Q:29:HIS:C	16:Q:31:LEU:H	2.25	0.40
23:Y:117:GLN:HE22	23:Y:664:GLN:HB3	1.86	0.40
7:H:90:GLY:O	11:L:7:ILE:HD13	2.21	0.40
20:A:643:C:H2'	20:A:644:G:C8	2.56	0.40
9:J:27:ALA:HB3	9:J:34:VAL:HG21	2.03	0.40
14:O:41:GLU:OE1	14:O:44:LYS:HE2	2.21	0.40
12:M:57:ARG:HB3	12:M:57:ARG:HE	1.51	0.40
15:P:10:GLY:HA2	20:A:624:C:H4'	2.04	0.40
20:A:1213:A:C8	20:A:1215:G:C5	3.08	0.40
20:A:1242:C:H2'	20:A:1243:C:H6	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:319:ASP:HA	23:Y:320:PRO:HD3	1.94	0.40
21:W:17:U:H5'	21:W:18:G:H4'	2.03	0.40
1:B:185:ILE:HD13	1:B:199:TYR:CD1	2.56	0.40
1:B:220:ASP:N	1:B:220:ASP:OD1	2.53	0.40
1:B:87:ARG:NH2	1:B:233:SER:H	2.20	0.40
20:A:1130:A:H61	20:A:1143:G:N2	2.19	0.40
20:A:1128:C:O2'	20:A:1130:A:N7	2.41	0.40
20:A:1350:A:H2'	20:A:1351:U:C6	2.57	0.40
15:P:80:PHE:HA	15:P:80:PHE:HD2	1.80	0.40
20:A:966:G:H2'	20:A:967:C:O4'	2.21	0.40
23:Y:353:ALA:O	23:Y:354:ARG:HG3	2.21	0.40
20:A:1420:C:H2'	20:A:1421:G:H5'	2.04	0.40
20:A:1260:C:OP1	20:A:1284:C:H4'	2.22	0.40
20:A:865:A:C2	20:A:918:A:H4'	2.56	0.40
7:H:109:ILE:HG12	7:H:111:ILE:HD13	2.03	0.40
6:G:27:ILE:HA	6:G:30:ILE:HD12	2.04	0.40
14:O:59:MET:HB2	14:O:59:MET:HE3	1.93	0.40
4:E:28:PHE:CE1	4:E:51:VAL:HG22	2.56	0.40
15:P:71:ARG:NH1	15:P:71:ARG:HB2	2.36	0.40
19:T:41:ILE:O	19:T:45:GLN:HB2	2.22	0.40
10:K:122:LYS:NZ	20:A:780:A:OP2	2.30	0.40
23:Y:435:ASP:HA	23:Y:436:PRO:HD2	1.82	0.40
20:A:269:C:H2'	20:A:270:A:O4'	2.20	0.40
23:Y:108:PHE:HZ	23:Y:122:TRP:CE3	2.39	0.40
6:G:99:LEU:HD22	6:G:103:TRP:HE1	1.87	0.40
20:A:1494:G:H2'	20:A:1495:U:C6	2.57	0.40
20:A:123:C:OP1	20:A:312:C:H5'	2.22	0.40
11:L:57:LYS:HA	11:L:65:GLU:O	2.22	0.40
1:B:51:LEU:HA	1:B:54:THR:HB	2.04	0.40
20:A:297:G:H2'	20:A:299:G:N7	2.37	0.40
23:Y:515:GLU:O	23:Y:564:LYS:HB3	2.21	0.40
23:Y:100:VAL:HG11	23:Y:314:PHE:CZ	2.57	0.40
20:A:720:C:H3'	20:A:721:G:H2'	2.03	0.40
20:A:364:A:H2'	20:A:365:U:O2	2.22	0.40
20:A:1316:G:H1'	20:A:1360:A:H2	1.87	0.40
20:A:243:A:H4'	20:A:244:U:H3'	2.03	0.40
3:D:155:LEU:HB3	3:D:158:ILE:HD13	2.03	0.40
20:A:1421:G:H2'	20:A:1422:G:O4'	2.22	0.40
8:I:107:ARG:NH2	20:A:1347:G:O4'	2.54	0.40
20:A:563:A:HO2'	20:A:566:G:HO2'	1.69	0.40
23:Y:20:HIS:CD2	23:Y:20:HIS:H	2.38	0.40
23:Y:98:MET:SD	23:Y:125:ALA:HB1	2.62	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1353:G:H2'	20:A:1354:C:C6	2.57	0.40
2:C:116:VAL:O	2:C:120:VAL:HG23	2.21	0.40
20:A:990:C:H2'	20:A:991:U:O4'	2.21	0.40
7:H:64:LYS:HG2	7:H:65:TYR:N	2.36	0.40
20:A:60:A:N3	20:A:61:G:H1'	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	233/235 (99%)	154 (66%)	51 (22%)	28 (12%)	1	11
2	C	205/207 (99%)	154 (75%)	32 (16%)	19 (9%)	1	18
3	D	206/208 (99%)	149 (72%)	31 (15%)	26 (13%)	0	10
4	E	149/151 (99%)	117 (78%)	22 (15%)	10 (7%)	2	28
5	F	99/101 (98%)	75 (76%)	15 (15%)	9 (9%)	1	18
6	G	153/155 (99%)	121 (79%)	25 (16%)	7 (5%)	4	39
7	H	136/138 (99%)	97 (71%)	27 (20%)	12 (9%)	1	19
8	I	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	5	44
9	J	97/99 (98%)	75 (77%)	13 (13%)	9 (9%)	1	18
10	K	117/119 (98%)	82 (70%)	21 (18%)	14 (12%)	1	11
11	L	123/125 (98%)	38 (31%)	52 (42%)	33 (27%)	0	1
12	M	123/125 (98%)	93 (76%)	20 (16%)	10 (8%)	1	21
13	N	58/60 (97%)	44 (76%)	7 (12%)	7 (12%)	1	11
14	O	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	21
15	P	82/84 (98%)	66 (80%)	15 (18%)	1 (1%)	19	75
16	Q	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	1	14
17	R	68/70 (97%)	51 (75%)	10 (15%)	7 (10%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	S	77/79 (98%)	41 (53%)	23 (30%)	13 (17%)	0	4
19	T	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	4	44
23	Y	663/687 (96%)	451 (68%)	138 (21%)	74 (11%)	1	13
24	U	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	2997/3063 (98%)	2119 (71%)	573 (19%)	305 (10%)	1	14

All (305) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	9	GLU
1	B	76	GLN
1	B	165	VAL
1	B	194	PRO
2	C	4	LYS
2	C	26	LYS
2	C	49	SER
3	D	4	TYR
3	D	5	ILE
3	D	24	GLU
3	D	28	SER
3	D	34	GLU
3	D	43	HIS
3	D	62	GLN
3	D	63	LYS
3	D	69	GLY
3	D	113	SER
3	D	156	GLU
4	E	36	ASP
4	E	125	SER
5	F	69	GLU
5	F	70	ASP
6	G	37	ASN
7	H	22	GLU
7	H	103	VAL
7	H	107	LEU
8	I	58	HIS
9	J	88	LEU
9	J	92	THR
10	K	42	TRP
10	K	109	VAL
10	K	120	ARG

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Mol	Chain	Res	Type
11	L	6	THR
11	L	7	ILE
11	L	13	LYS
11	L	39	VAL
11	L	43	VAL
11	L	48	PRO
11	L	55	VAL
11	L	78	GLN
11	L	94	PRO
11	L	102	ARG
11	L	104	VAL
11	L	107	ALA
11	L	115	LYS
11	L	123	LYS
12	M	3	ARG
12	M	6	GLY
12	M	113	PRO
13	N	3	ARG
14	O	19	PRO
15	P	28	ARG
16	Q	28	PRO
16	Q	55	ASP
16	Q	69	LYS
17	R	36	ASN
17	R	37	VAL
17	R	45	SER
18	S	37	ARG
18	S	38	SER
18	S	53	ASN
18	S	70	LYS
19	T	74	LYS
23	Y	22	ASP
23	Y	84	THR
23	Y	87	HIS
23	Y	92	ILE
23	Y	171	GLU
23	Y	224	ASP
23	Y	244	ALA
23	Y	266	ASN
23	Y	330	VAL
23	Y	331	TYR
23	Y	384	ILE

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Mol	Chain	Res	Type
23	Y	395	PRO
23	Y	448	GLN
23	Y	518	PRO
23	Y	527	ASN
23	Y	565	VAL
23	Y	568	TYR
23	Y	628	ARG
23	Y	659	LEU
23	Y	681	LYS
1	B	15	VAL
1	B	34	ALA
1	B	129	GLU
1	B	186	ALA
1	B	195	ASP
1	B	229	VAL
2	C	44	GLU
2	C	48	TYR
2	C	51	GLY
2	C	60	ALA
2	C	73	PRO
2	C	76	VAL
2	C	130	VAL
2	C	161	GLU
3	D	27	TYR
3	D	44	GLY
3	D	134	ASP
3	D	186	LEU
4	E	6	PHE
4	E	85	GLY
4	E	104	ALA
5	F	85	VAL
6	G	15	ASP
6	G	80	VAL
7	H	27	PRO
7	H	92	ARG
7	H	134	ILE
9	J	51	ARG
9	J	55	LYS
9	J	59	SER
10	K	12	ARG
10	K	36	ASP
10	K	43	SER

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Mol	Chain	Res	Type
10	K	90	GLY
10	K	91	ARG
11	L	19	ARG
11	L	31	PRO
11	L	34	ARG
11	L	35	GLY
11	L	37	CYS
11	L	50	SER
11	L	66	VAL
11	L	80	HIS
11	L	116	SER
11	L	121	GLY
11	L	125	PRO
12	M	12	ASN
12	M	101	GLN
16	Q	12	SER
16	Q	34	LYS
16	Q	53	LEU
18	S	45	VAL
18	S	66	MET
18	S	67	VAL
19	T	71	THR
19	T	94	ALA
23	Y	20	HIS
23	Y	21	ILE
23	Y	25	LYS
23	Y	39	ILE
23	Y	40	HIS
23	Y	66	THR
23	Y	86	GLY
23	Y	129	LYS
23	Y	205	TYR
23	Y	258	VAL
23	Y	297	GLU
23	Y	436	PRO
23	Y	471	LYS
23	Y	475	ASN
23	Y	476	VAL
23	Y	521	SER
23	Y	555	LEU
23	Y	615	GLU
23	Y	631	ILE

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Mol	Chain	Res	Type
23	Y	658	ASP
23	Y	661	SER
23	Y	668	SER
1	B	17	PHE
1	B	20	GLU
1	B	94	ASN
1	B	95	GLN
1	B	100	GLY
1	B	175	ARG
1	B	183	PRO
1	B	235	SER
2	C	112	SER
2	C	162	GLN
3	D	21	LEU
3	D	88	VAL
3	D	89	THR
3	D	197	PRO
4	E	126	ARG
5	F	14	LEU
5	F	96	PRO
6	G	10	ARG
6	G	100	ALA
7	H	90	GLY
7	H	99	GLU
8	I	24	GLY
9	J	14	LYS
9	J	37	PRO
9	J	57	LYS
11	L	18	VAL
11	L	64	TYR
11	L	69	TYR
11	L	96	VAL
12	M	99	ARG
12	M	107	ALA
13	N	58	LYS
18	S	65	ASN
18	S	77	THR
18	S	80	TYR
23	Y	6	GLU
23	Y	91	THR
23	Y	111	SER
23	Y	128	TYR

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Mol	Chain	Res	Type
23	Y	148	LEU
23	Y	203	GLU
23	Y	245	ALA
23	Y	257	PRO
23	Y	320	PRO
23	Y	437	THR
23	Y	498	ILE
23	Y	574	GLU
23	Y	660	ARG
1	B	54	THR
1	B	157	ARG
1	B	184	VAL
1	B	215	LEU
1	B	237	ALA
2	C	85	ARG
2	C	96	GLY
3	D	30	LYS
3	D	33	MET
5	F	34	GLY
6	G	12	LEU
6	G	33	ASP
7	H	2	LEU
7	H	100	ILE
8	I	12	GLU
8	I	119	ALA
10	K	15	ALA
10	K	35	PRO
11	L	127	GLU
12	M	10	PRO
12	M	21	TYR
12	M	117	VAL
13	N	13	THR
13	N	27	CYS
14	O	20	GLY
14	O	24	SER
14	O	47	LYS
16	Q	33	GLY
16	Q	71	PHE
17	R	55	ARG
18	S	40	ILE
23	Y	304	ASP
23	Y	341	VAL

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Mol	Chain	Res	Type
23	Y	381	LYS
23	Y	531	GLY
23	Y	567	LEU
23	Y	600	VAL
1	B	67	THR
1	B	103	THR
2	C	75	VAL
3	D	84	LYS
3	D	204	ILE
4	E	100	VAL
4	E	106	PRO
5	F	38	GLU
8	I	101	PHE
9	J	32	ALA
10	K	111	ASP
11	L	79	GLU
13	N	15	LYS
14	O	18	PHE
17	R	33	ASP
17	R	87	ARG
23	Y	206	LEU
23	Y	225	GLU
23	Y	347	GLY
23	Y	532	GLY
23	Y	533	VAL
23	Y	688	ILE
1	B	230	VAL
2	C	13	GLY
3	D	7	PRO
3	D	47	ARG
4	E	65	ASN
7	H	72	PRO
11	L	93	LEU
14	O	5	LYS
23	Y	360	ALA
23	Y	361	ASN
2	C	109	PRO
2	C	174	PRO
3	D	23	GLY
4	E	74	GLY
5	F	37	VAL
7	H	97	VAL

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Mol	Chain	Res	Type
10	K	113	PRO
14	O	23	GLY
16	Q	30	PRO
18	S	46	GLY
23	Y	116	PRO
23	Y	638	GLY
23	Y	680	PRO
10	K	14	VAL
23	Y	65	ILE
23	Y	301	ILE
1	B	164	VAL
1	B	174	VAL
5	F	51	PRO
13	N	14	PRO
18	S	59	PRO
10	K	48	ILE
11	L	95	GLY
13	N	18	VAL
16	Q	64	PRO
17	R	39	VAL
19	T	47	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	203/203 (100%)	164 (81%)	39 (19%)	2	12
2	C	161/161 (100%)	132 (82%)	29 (18%)	2	15
3	D	180/180 (100%)	145 (81%)	35 (19%)	2	12
4	E	116/116 (100%)	93 (80%)	23 (20%)	2	11
5	F	90/90 (100%)	78 (87%)	12 (13%)	6	31
6	G	126/126 (100%)	113 (90%)	13 (10%)	10	47
7	H	119/119 (100%)	98 (82%)	21 (18%)	3	16
8	I	98/98 (100%)	82 (84%)	16 (16%)	3	21
9	J	89/89 (100%)	75 (84%)	14 (16%)	4	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	K	90/90 (100%)	71 (79%)	19 (21%)	1	9
11	L	104/104 (100%)	77 (74%)	27 (26%)	1	5
12	M	100/100 (100%)	83 (83%)	17 (17%)	3	18
13	N	49/49 (100%)	43 (88%)	6 (12%)	7	36
14	O	79/79 (100%)	71 (90%)	8 (10%)	11	48
15	P	72/72 (100%)	66 (92%)	6 (8%)	16	59
16	Q	95/95 (100%)	81 (85%)	14 (15%)	4	26
17	R	61/61 (100%)	51 (84%)	10 (16%)	3	20
18	S	69/69 (100%)	55 (80%)	14 (20%)	2	11
19	T	76/76 (100%)	64 (84%)	12 (16%)	4	23
23	Y	563/579 (97%)	470 (84%)	93 (16%)	3	20
24	U	2/2 (100%)	2 (100%)	0	100	100
All	All	2542/2558 (99%)	2114 (83%)	428 (17%)	3	19

All (428) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	VAL
1	B	9	GLU
1	B	12	GLU
1	B	15	VAL
1	B	17	PHE
1	B	36	ARG
1	B	40	HIS
1	B	42	ILE
1	B	49	GLU
1	B	69	LEU
1	B	70	PHE
1	B	74	LYS
1	B	96	ARG
1	B	103	THR
1	B	115	LEU
1	B	128	GLU
1	B	134	GLU
1	B	137	ARG
1	B	140	HIS
1	B	141	GLU
1	B	142	LEU

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Mol	Chain	Res	Type
1	B	145	LEU
1	B	157	ARG
1	B	160	ASP
1	B	162	ILE
1	B	163	PHE
1	B	168	THR
1	B	172	ILE
1	B	175	ARG
1	B	185	ILE
1	B	187	LEU
1	B	190	THR
1	B	191	ASP
1	B	198	ASP
1	B	212	GLN
1	B	213	LEU
1	B	226	ARG
1	B	230	VAL
1	B	239	VAL
2	C	4	LYS
2	C	5	ILE
2	C	6	HIS
2	C	10	PHE
2	C	15	THR
2	C	22	TRP
2	C	32	LEU
2	C	38	ARG
2	C	57	ILE
2	C	67	THR
2	C	76	VAL
2	C	83	ARG
2	C	84	ILE
2	C	101	LEU
2	C	110	ASN
2	C	124	ILE
2	C	125	GLU
2	C	128	PHE
2	C	132	ARG
2	C	134	ILE
2	C	136	GLN
2	C	153	VAL
2	C	167	TRP
2	C	175	LEU

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Mol	Chain	Res	Type
2	C	176	HIS
2	C	184	TYR
2	C	196	LEU
2	C	204	LEU
2	C	208	ILE
3	D	3	ARG
3	D	5	ILE
3	D	10	ARG
3	D	19	LEU
3	D	30	LYS
3	D	53	ASP
3	D	54	TYR
3	D	57	ARG
3	D	61	LYS
3	D	66	ARG
3	D	72	GLU
3	D	80	GLU
3	D	86	LYS
3	D	89	THR
3	D	96	LEU
3	D	102	ASP
3	D	107	ARG
3	D	127	THR
3	D	131	ARG
3	D	132	ARG
3	D	134	ASP
3	D	138	TYR
3	D	140	VAL
3	D	141	ARG
3	D	150	GLU
3	D	156	GLU
3	D	170	VAL
3	D	177	ASP
3	D	178	VAL
3	D	181	MET
3	D	187	ARG
3	D	191	ARG
3	D	193	ASP
3	D	196	LEU
3	D	200	GLU
4	E	11	ILE
4	E	12	LEU

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Mol	Chain	Res	Type
4	E	26	PHE
4	E	31	LEU
4	E	34	VAL
4	E	36	ASP
4	E	41	VAL
4	E	47	LYS
4	E	51	VAL
4	E	63	ARG
4	E	64	ARG
4	E	72	GLN
4	E	75	THR
4	E	78	HIS
4	E	80	ILE
4	E	91	LEU
4	E	98	THR
4	E	100	VAL
4	E	107	ARG
4	E	119	LEU
4	E	125	SER
4	E	139	LEU
4	E	145	LYS
5	F	2	ARG
5	F	13	ASN
5	F	16	GLN
5	F	31	GLU
5	F	33	TYR
5	F	61	LEU
5	F	63	TYR
5	F	64	GLN
5	F	67	MET
5	F	80	ARG
5	F	89	MET
5	F	98	LEU
6	G	5	ARG
6	G	11	GLN
6	G	13	GLN
6	G	24	THR
6	G	32	ARG
6	G	56	GLN
6	G	68	ASN
6	G	79	ARG
6	G	80	VAL

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Mol	Chain	Res	Type
6	G	94	ARG
6	G	97	GLN
6	G	122	HIS
6	G	149	ARG
7	H	21	LYS
7	H	31	PHE
7	H	37	ARG
7	H	44	PHE
7	H	48	TYR
7	H	51	VAL
7	H	59	LEU
7	H	62	TYR
7	H	63	LEU
7	H	69	ARG
7	H	73	ASP
7	H	82	HIS
7	H	92	ARG
7	H	95	VAL
7	H	102	ARG
7	H	103	VAL
7	H	107	LEU
7	H	111	ILE
7	H	112	LEU
7	H	120	THR
7	H	138	TRP
8	I	25	LYS
8	I	28	VAL
8	I	40	LEU
8	I	66	ARG
8	I	79	LEU
8	I	85	LEU
8	I	88	TYR
8	I	95	LYS
8	I	97	LYS
8	I	99	LEU
8	I	102	LEU
8	I	104	ARG
8	I	111	ARG
8	I	113	LYS
8	I	121	ARG
8	I	128	ARG
9	J	6	ILE

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Mol	Chain	Res	Type
9	J	15	THR
9	J	16	LEU
9	J	38	ILE
9	J	43	ARG
9	J	55	LYS
9	J	70	ARG
9	J	73	ASP
9	J	75	ILE
9	J	78	ASN
9	J	79	ARG
9	J	83	GLU
9	J	96	ILE
9	J	101	VAL
10	K	25	TYR
10	K	29	ILE
10	K	31	THR
10	K	34	ASP
10	K	40	ILE
10	K	41	THR
10	K	48	ILE
10	K	57	THR
10	K	73	MET
10	K	77	MET
10	K	80	VAL
10	K	81	ASP
10	K	84	VAL
10	K	98	LEU
10	K	110	ASP
10	K	116	HIS
10	K	117	ASN
10	K	120	ARG
10	K	124	LYS
11	L	18	VAL
11	L	20	LYS
11	L	24	VAL
11	L	33	ARG
11	L	38	THR
11	L	42	THR
11	L	43	VAL
11	L	44	THR
11	L	53	ARG
11	L	54	LYS

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Mol	Chain	Res	Type
11	L	55	VAL
11	L	59	ARG
11	L	61	THR
11	L	67	THR
11	L	70	ILE
11	L	75	HIS
11	L	76	ASN
11	L	79	GLU
11	L	85	ILE
11	L	90	VAL
11	L	92	ASP
11	L	96	VAL
11	L	102	ARG
11	L	105	TYR
11	L	116	SER
11	L	120	TYR
11	L	127	GLU
12	M	8	GLU
12	M	16	ASP
12	M	21	TYR
12	M	27	LYS
12	M	56	LEU
12	M	61	GLU
12	M	67	GLU
12	M	71	ARG
12	M	73	GLU
12	M	82	MET
12	M	83	ASP
12	M	108	ARG
12	M	110	ARG
12	M	115	LYS
12	M	120	LYS
12	M	121	LYS
12	M	125	ARG
13	N	7	ILE
13	N	21	TYR
13	N	35	ARG
13	N	40	CYS
13	N	41	ARG
13	N	61	TRP
14	O	5	LYS
14	O	10	LYS

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Mol	Chain	Res	Type
14	O	31	LEU
14	O	38	ARG
14	O	41	GLU
14	O	82	ILE
14	O	85	LEU
14	O	88	ARG
15	P	28	ARG
15	P	29	ASP
15	P	57	ARG
15	P	67	THR
15	P	69	THR
15	P	71	ARG
16	Q	5	VAL
16	Q	6	LEU
16	Q	7	THR
16	Q	16	GLN
16	Q	24	GLU
16	Q	32	TYR
16	Q	48	GLU
16	Q	52	LYS
16	Q	59	ILE
16	Q	63	ARG
16	Q	66	SER
16	Q	69	LYS
16	Q	74	LEU
16	Q	93	GLN
17	R	19	LYS
17	R	29	PHE
17	R	32	ARG
17	R	37	VAL
17	R	43	PHE
17	R	47	THR
17	R	53	ARG
17	R	54	ARG
17	R	69	THR
17	R	83	GLU
18	S	5	LEU
18	S	6	LYS
18	S	7	LYS
18	S	23	ASN
18	S	25	LYS
18	S	28	LYS

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Mol	Chain	Res	Type
18	S	32	LYS
18	S	47	HIS
18	S	51	VAL
18	S	58	VAL
18	S	61	TYR
18	S	62	ILE
18	S	79	THR
18	S	81	ARG
19	T	13	LEU
19	T	25	ARG
19	T	35	THR
19	T	36	LEU
19	T	50	GLU
19	T	54	LYS
19	T	56	MET
19	T	57	ARG
19	T	71	THR
19	T	73	HIS
19	T	74	LYS
19	T	80	ARG
23	Y	20	HIS
23	Y	29	THR
23	Y	30	GLU
23	Y	35	TYR
23	Y	36	THR
23	Y	72	CYS
23	Y	73	PHE
23	Y	87	HIS
23	Y	92	ILE
23	Y	93	GLU
23	Y	112	GLN
23	Y	119	GLU
23	Y	121	VAL
23	Y	126	GLU
23	Y	132	ARG
23	Y	133	ILE
23	Y	137	ASN
23	Y	139	MET
23	Y	140	ASP
23	Y	146	LEU
23	Y	157	LEU
23	Y	165	GLN

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Mol	Chain	Res	Type
23	Y	170	ARG
23	Y	174	PHE
23	Y	178	ILE
23	Y	186	TYR
23	Y	188	TYR
23	Y	191	ASP
23	Y	197	ARG
23	Y	199	ILE
23	Y	210	ARG
23	Y	227	ILE
23	Y	229	LEU
23	Y	240	GLU
23	Y	252	ASP
23	Y	255	ILE
23	Y	260	LEU
23	Y	264	LEU
23	Y	266	ASN
23	Y	271	LEU
23	Y	273	LEU
23	Y	282	SER
23	Y	299	VAL
23	Y	302	HIS
23	Y	312	LEU
23	Y	314	PHE
23	Y	319	ASP
23	Y	321	TYR
23	Y	328	ILE
23	Y	340	TYR
23	Y	341	VAL
23	Y	342	TYR
23	Y	344	THR
23	Y	352	VAL
23	Y	358	MET
23	Y	364	GLU
23	Y	368	GLU
23	Y	393	ASP
23	Y	404	VAL
23	Y	406	GLU
23	Y	428	LEU
23	Y	440	VAL
23	Y	454	MET
23	Y	456	GLU

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Mol	Chain	Res	Type
23	Y	460	GLU
23	Y	464	ASP
23	Y	468	ARG
23	Y	475	ASN
23	Y	487	ILE
23	Y	488	THR
23	Y	498	ILE
23	Y	499	ARG
23	Y	504	ARG
23	Y	506	GLN
23	Y	507	TYR
23	Y	512	ILE
23	Y	517	LEU
23	Y	525	PHE
23	Y	526	VAL
23	Y	529	ILE
23	Y	556	ILE
23	Y	563	ILE
23	Y	572	TYR
23	Y	574	GLU
23	Y	580	MET
23	Y	603	GLU
23	Y	610	VAL
23	Y	614	GLU
23	Y	617	MET
23	Y	641	GLN
23	Y	647	VAL
23	Y	666	ARG
23	Y	676	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	69	HIS
2	C	102	ASN
3	D	77	ASN
5	F	100	ASN
6	G	97	GLN
7	H	78	GLN
8	I	117	HIS
10	K	62	GLN
10	K	93	GLN

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Mol	Chain	Res	Type
10	K	116	HIS
11	L	49	ASN
11	L	76	ASN
15	P	16	HIS
17	R	63	GLN
23	Y	20	HIS
23	Y	117	GLN
23	Y	137	ASN
23	Y	190	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	A	1510/1511 (99%)	305 (20%)	17 (1%)
21	W	76/77 (98%)	23 (30%)	1 (1%)
22	V	22/23 (95%)	8 (36%)	1 (4%)
All	All	1608/1611 (99%)	336 (20%)	19 (1%)

All (336) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	A	6	G
20	A	9	G
20	A	13	U
20	A	15	G
20	A	29	G
20	A	32	A
20	A	39	G
20	A	47	C
20	A	48	C
20	A	50	A
20	A	51	A
20	A	68(H)	G
20	A	68(L)	U
20	A	68(M)	U
20	A	68(P)	C
20	A	68(W)	G
20	A	106	C
20	A	108	G
20	A	109	A
20	A	116	A

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Mol	Chain	Res	Type
20	A	121	C
20	A	122	G
20	A	129(A)	G
20	A	131	C
20	A	144	G
20	A	152	A
20	A	163	C
20	A	175	C
20	A	179	A
20	A	186(G)	C
20	A	186(I)	U
20	A	186(L)	G
20	A	195	A
20	A	197	A
20	A	201(C)	U
20	A	216	G
20	A	220	G
20	A	231	G
20	A	244	U
20	A	245	C
20	A	247	G
20	A	251	G
20	A	253	U
20	A	264	U
20	A	267	C
20	A	273	A
20	A	279	A
20	A	280	C
20	A	281	G
20	A	289	G
20	A	306	G
20	A	309	G
20	A	316	G
20	A	321	A
20	A	328	C
20	A	329	A
20	A	332	G
20	A	338	A
20	A	345	C
20	A	347	G
20	A	352	C
20	A	353	A

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Mol	Chain	Res	Type
20	A	354	G
20	A	357	G
20	A	367	U
20	A	372	C
20	A	373	A
20	A	384	G
20	A	390	C
20	A	397	A
20	A	398	C
20	A	407	G
20	A	411	A
20	A	412	A
20	A	413	G
20	A	414	A
20	A	422	C
20	A	423	G
20	A	424	G
20	A	430	A
20	A	440	A
20	A	452	A
20	A	453	A
20	A	458	C
20	A	458(B)	A
20	A	481	G
20	A	485	G
20	A	492	G
20	A	495	A
20	A	497	A
20	A	498	U
20	A	505	G
20	A	509	A
20	A	511	C
20	A	514	C
20	A	518	C
20	A	519	C
20	A	521	G
20	A	522	C
20	A	524	G
20	A	527	G
20	A	531	U
20	A	532	A
20	A	533	A

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Mol	Chain	Res	Type
20	A	534	U
20	A	538	G
20	A	547	A
20	A	559	A
20	A	560	U
20	A	562	C
20	A	564	C
20	A	567	G
20	A	568	G
20	A	572	A
20	A	573	A
20	A	574	A
20	A	575	G
20	A	576	G
20	A	577	G
20	A	579	G
20	A	596	C
20	A	653	A
20	A	661	G
20	A	665	A
20	A	673	G
20	A	685	G
20	A	688	G
20	A	703	G
20	A	713	G
20	A	723	U
20	A	724	G
20	A	730	G
20	A	731	G
20	A	733	A
20	A	734	G
20	A	737	A
20	A	740	U
20	A	749	C
20	A	754	C
20	A	755	G
20	A	777	A
20	A	793	U
20	A	794	A
20	A	807	A
20	A	811	C
20	A	812	C

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Mol	Chain	Res	Type
20	A	816	A
20	A	817	C
20	A	818	G
20	A	819	A
20	A	821	G
20	A	827	U
20	A	828	A
20	A	834	C
20	A	838(A)	U
20	A	838(B)	C
20	A	838(C)	U
20	A	848	C
20	A	859	A
20	A	867	G
20	A	869	G
20	A	870	U
20	A	873	A
20	A	874	G
20	A	877	C
20	A	897	C
20	A	902	G
20	A	907	A
20	A	916	G
20	A	923	A
20	A	926	G
20	A	927	G
20	A	934	C
20	A	935	A
20	A	960	U
20	A	961	U
20	A	962	C
20	A	966	G
20	A	969	A
20	A	971	G
20	A	972	C
20	A	974	A
20	A	976	G
20	A	977	A
20	A	978	A
20	A	979	C
20	A	980	C
20	A	983	A

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Mol	Chain	Res	Type
20	A	992	U
20	A	993	G
20	A	1004	A
20	A	1025	U
20	A	1045	C
20	A	1046	A
20	A	1047	G
20	A	1049	U
20	A	1054	C
20	A	1055	A
20	A	1065	U
20	A	1066	C
20	A	1067	A
20	A	1069	C
20	A	1081	G
20	A	1085	U
20	A	1094	G
20	A	1095	U
20	A	1097	C
20	A	1101	A
20	A	1102	A
20	A	1125	U
20	A	1126	U
20	A	1129	C
20	A	1130	A
20	A	1137	C
20	A	1138	G
20	A	1139	G
20	A	1140	C
20	A	1146	A
20	A	1152	A
20	A	1154	G
20	A	1158	C
20	A	1159	U
20	A	1181	G
20	A	1187	G
20	A	1191	A
20	A	1196	U
20	A	1197	G
20	A	1198	G
20	A	1200	C
20	A	1201	A

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Mol	Chain	Res	Type
20	A	1203	C
20	A	1204	A
20	A	1212	U
20	A	1213	A
20	A	1214	C
20	A	1220	G
20	A	1225	A
20	A	1226	C
20	A	1227	A
20	A	1238	A
20	A	1239	A
20	A	1247	U
20	A	1249	C
20	A	1256	A
20	A	1257	U
20	A	1260	C
20	A	1275	A
20	A	1279	A
20	A	1280	A
20	A	1281	U
20	A	1283	G
20	A	1287	A
20	A	1300	G
20	A	1301	U
20	A	1302	U
20	A	1303	C
20	A	1305	G
20	A	1311	G
20	A	1317	C
20	A	1320	C
20	A	1322	C
20	A	1331	G
20	A	1338	G
20	A	1339	A
20	A	1347	G
20	A	1362(A)	C
20	A	1364	U
20	A	1370	G
20	A	1377	A
20	A	1397	C
20	A	1398	A
20	A	1402	C

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Mol	Chain	Res	Type
20	A	1403	C
20	A	1406	U
20	A	1413	A
20	A	1419	G
20	A	1440(C)	G
20	A	1440(D)	A
20	A	1440(E)	G
20	A	1440(I)	A
20	A	1440(J)	C
20	A	1440(K)	G
20	A	1440(L)	G
20	A	1475	G
20	A	1489	G
20	A	1492	A
20	A	1493	A
20	A	1494	G
20	A	1497	G
20	A	1499	A
20	A	1502	A
20	A	1504	G
20	A	1505	G
20	A	1506	U
20	A	1517	G
20	A	1519	A
20	A	1520	G
20	A	1529	G
20	A	1530	G
20	A	1532	U
20	A	1533	C
20	A	1534	A
20	A	1535	C
20	A	1536	C
20	A	1538	C
21	W	8	U
21	W	16	U
21	W	17	U
21	W	18	G
21	W	19	G
21	W	20	U
21	W	20(A)	U
21	W	21	A
21	W	22	G

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Mol	Chain	Res	Type
21	W	25	C
21	W	30	C
21	W	36	U
21	W	42	U
21	W	46	G
21	W	47	U
21	W	48	C
21	W	49	A
21	W	50	C
21	W	51	A
21	W	58	A
21	W	59	A
21	W	60	U
21	W	61	C
22	V	5	A
22	V	12	A
22	V	15	A
22	V	16	A
22	V	18	G
22	V	19	G
22	V	23	A
22	V	24	A

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	A	115	G
20	A	243	A
20	A	266	G
20	A	281	G
20	A	328	C
20	A	429	U
20	A	484	G
20	A	687	A
20	A	739	C
20	A	748	C
20	A	992	U
20	A	1064	G
20	A	1101	A
20	A	1145	C
20	A	1504	G
20	A	1532	U

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Mol	Chain	Res	Type
20	A	1537	U
21	W	41	A
22	V	18	G

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	KBE	U	1	24	8,8,9	8.27	1 (12%)	6,8,10	0.70	0
24	DPP	U	2	24	5,5,6	6.96	1 (20%)	3,5,7	2.10	1 (33%)
24	UAL	U	5	24	7,8,9	1.32	1 (14%)	6,9,11	1.44	1 (16%)
24	5OH	U	6	24	12,12,13	5.61	4 (33%)	13,16,18	2.23	3 (23%)

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	KBE	U	1	24	-	0/6/7/8	0/0/0/0
24	DPP	U	2	24	-	0/2/4/6	0/0/0/0
24	UAL	U	5	24	-	0/3/7/9	0/0/0/0
24	5OH	U	6	24	-	0/2/18/20	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	1	KBE	O-C	23.33	1.27	1.11
24	U	6	5OH	O-C	17.99	1.23	1.11
24	U	2	DPP	O-C	15.46	1.22	1.11
24	U	6	5OH	CQ-NP	5.73	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	6	5OH	CA-C	3.71	1.55	1.48
24	U	5	UAL	CA-N	-2.34	1.31	1.35
24	U	6	5OH	CQ-NR	2.27	1.40	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	U	6	5OH	CR-CB-CA	4.35	117.65	112.53
24	U	6	5OH	CR-CS-NR	4.28	120.78	108.18
24	U	6	5OH	CR-CB-NP	3.93	114.43	108.69
24	U	2	DPP	CB-CA-N	-2.62	102.70	111.50
24	U	5	UAL	CB-CA-N	2.15	128.00	123.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z  > 2$
25	FUA	Y	701	-	40,40,40	1.80	8 (20%)	64,64,64	1.88	13 (20%)
26	GDP	Y	702	-	30,30,30	1.20	2 (6%)	44,47,47	2.06	10 (22%)

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
25	FUA	Y	701	-	-	1/18/92/92	0/0/4/4
26	GDP	Y	702	-	-	0/16/32/32	0/1/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	701	FUA	C17-C22	4.57	1.39	1.34
25	Y	701	FUA	C29-C22	4.50	1.53	1.47
25	Y	701	FUA	C23-C22	-4.09	1.40	1.51
25	Y	701	FUA	C23-C24	-4.01	1.39	1.53
25	Y	701	FUA	C24-C25	-3.72	1.39	1.50
26	Y	702	GDP	C4-N9	-2.89	1.33	1.37
26	Y	702	GDP	C2-N1	2.45	1.40	1.36
25	Y	701	FUA	C14-C8	-2.43	1.53	1.58
25	Y	701	FUA	O6-C3	-2.37	1.38	1.43
25	Y	701	FUA	C25-C26	2.13	1.39	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	702	GDP	C6-C5-N7	-6.72	133.24	134.14
25	Y	701	FUA	C13-C12-C11	-5.87	103.73	112.00
25	Y	701	FUA	C24-C23-C22	5.55	125.63	111.93
26	Y	702	GDP	C2-N3-C4	4.54	121.47	115.09
26	Y	702	GDP	O4'-C1'-N9	4.30	112.44	108.44
26	Y	702	GDP	PA-O3A-PB	-4.21	119.34	131.68
25	Y	701	FUA	C23-C22-C17	-4.06	115.27	123.08
25	Y	701	FUA	C16-O2-C31	-3.85	110.99	117.13
25	Y	701	FUA	C23-C22-C29	3.56	122.99	115.50
26	Y	702	GDP	C5-C4-N3	-3.54	120.81	125.94
26	Y	702	GDP	C4'-O4'-C1'	-3.54	105.90	109.75
26	Y	702	GDP	N3-C4-N9	3.53	132.09	126.91
25	Y	701	FUA	C10-C9-C11	3.34	120.05	114.55
25	Y	701	FUA	C1-C10-C5	3.20	112.30	107.90
25	Y	701	FUA	O2-C31-C32	2.98	116.73	111.12
26	Y	702	GDP	C4-C5-N7	-2.76	107.16	109.52
25	Y	701	FUA	C21-C14-C8	-2.53	109.53	112.36
26	Y	702	GDP	O4'-C1'-C2'	-2.43	103.05	106.77
25	Y	701	FUA	C1-C2-C3	-2.41	106.51	111.45
26	Y	702	GDP	N2-C2-N1	2.33	120.43	117.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	701	FUA	O5-C29-O4	-2.14	118.57	123.62
25	Y	701	FUA	C7-C8-C14	-2.08	108.71	110.72
25	Y	701	FUA	C23-C24-C25	2.02	117.38	111.62

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	Y	701	FUA	C16-C17-C22-C29

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.