Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:41 PM GMT

PDB ID	:	4YHH
Title	:	Crystal structure of the 30S ribosomal subunit from Thermus thermophilus in complex with tigecycline
Authors	:	Schedlbauer, A.; Kaminishi, T.; Ochoa-Lizarralde, B.; Dhimole, N.; Zhou, S.; Lopez-Alonso, J.P.; Connell, S.R.; Fucini, P.
Deposited on	:	2015-02-27
Resolution	:	3.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

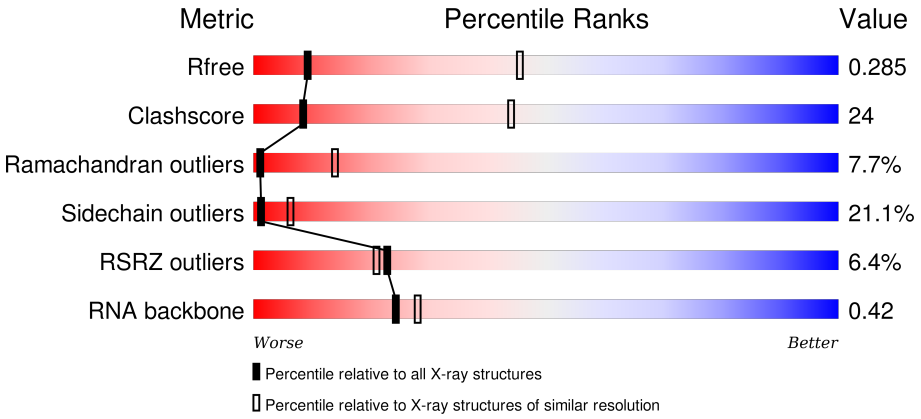
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.42 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)
RNA backbone	2183	1042 (4.02-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1507	23% 48% 25% .
2	B	226	6% 33% 48% 17% .
3	C	206	% 39% 49% 12%
4	D	208	6% 28% 53% 16% .

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Mol	Chain	Length	Quality of chain
5	E	157	13% 34% 45% 20%
6	F	101	5% 27% 45% 27%
7	G	155	5% 49% 44% 6%
8	H	138	3% 30% 47% 21%
9	I	127	6% 50% 38% 12%
10	J	99	18% 45% 48% 6%
11	K	115	8% 46% 43% 10%
12	L	124	19% 42% 47% 10%
13	M	119	24% 49% 41% 9%
14	N	60	3% 32% 50% 18%
15	O	88	33% 51% 16%
16	P	85	13% 40% 51% 9%
17	Q	104	33% 44% 38% 16%
18	R	73	25% 37% 41% 21%
19	S	83	12% 57% 30% 13%
20	T	99	11% 48% 42% 9%
21	V	24	21% 58% 17% 17% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1632	-	-	-	X
23	MG	A	1633	-	-	-	X
23	MG	A	1635	-	-	-	X
23	MG	A	1643	-	-	-	X
23	MG	A	1669	-	-	-	X
23	MG	A	1677	-	-	-	X
23	MG	A	1694	-	-	-	X
23	MG	A	1696	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1697	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 51732 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1507	32392	14418	6001	10467	1506	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	226	1842	1174	332	331	5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	206	1613	1016	314	282	1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	157	1199	754	228	213	4	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	0
			854	531	160	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	119	Total	C	N	O	S	0	0	0
			947	585	195	165	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	85	Total	C	N	O	S	0	0	0
			717	452	144	120	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	160	148	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			598	381	118	99			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	83	Total	C	N	O	S	0	0	0
			666	424	124	116	2			

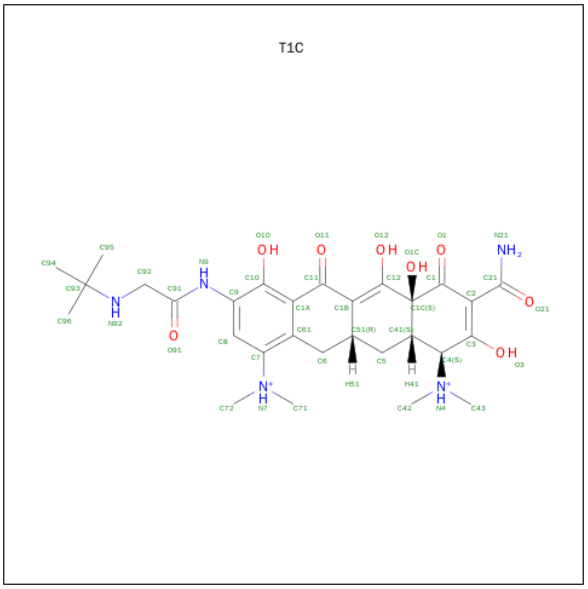
- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	V	24	Total C N O 209 128 50 31	0	0	0

- Molecule 22 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C N O 42 29 5 8	0	0

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	102	Total Mg 102 102	0	0
23	E	1	Total Mg 1 1	0	0

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

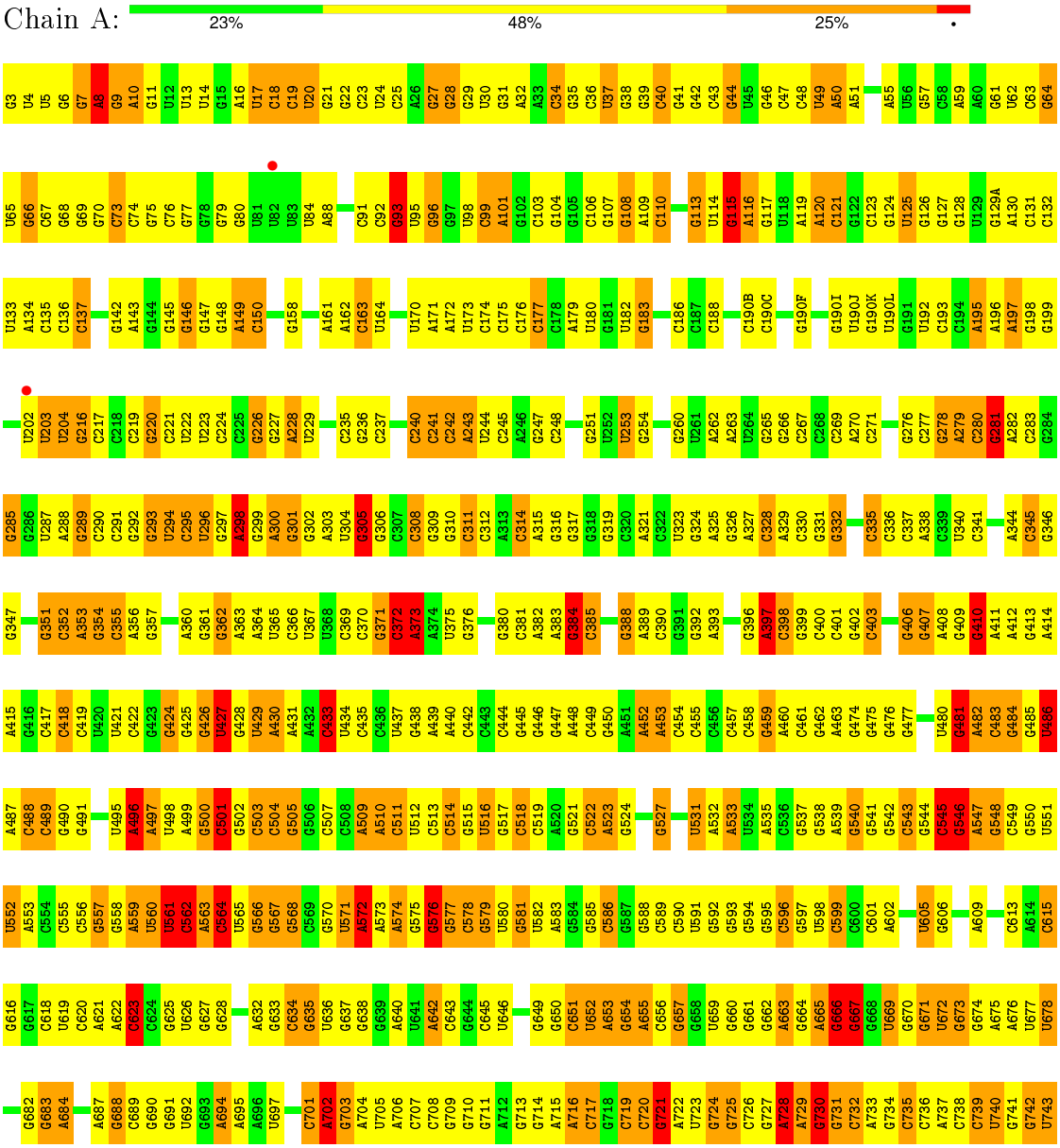
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	D	1	Total Zn 1 1	0	0
24	N	1	Total Zn 1 1	0	0

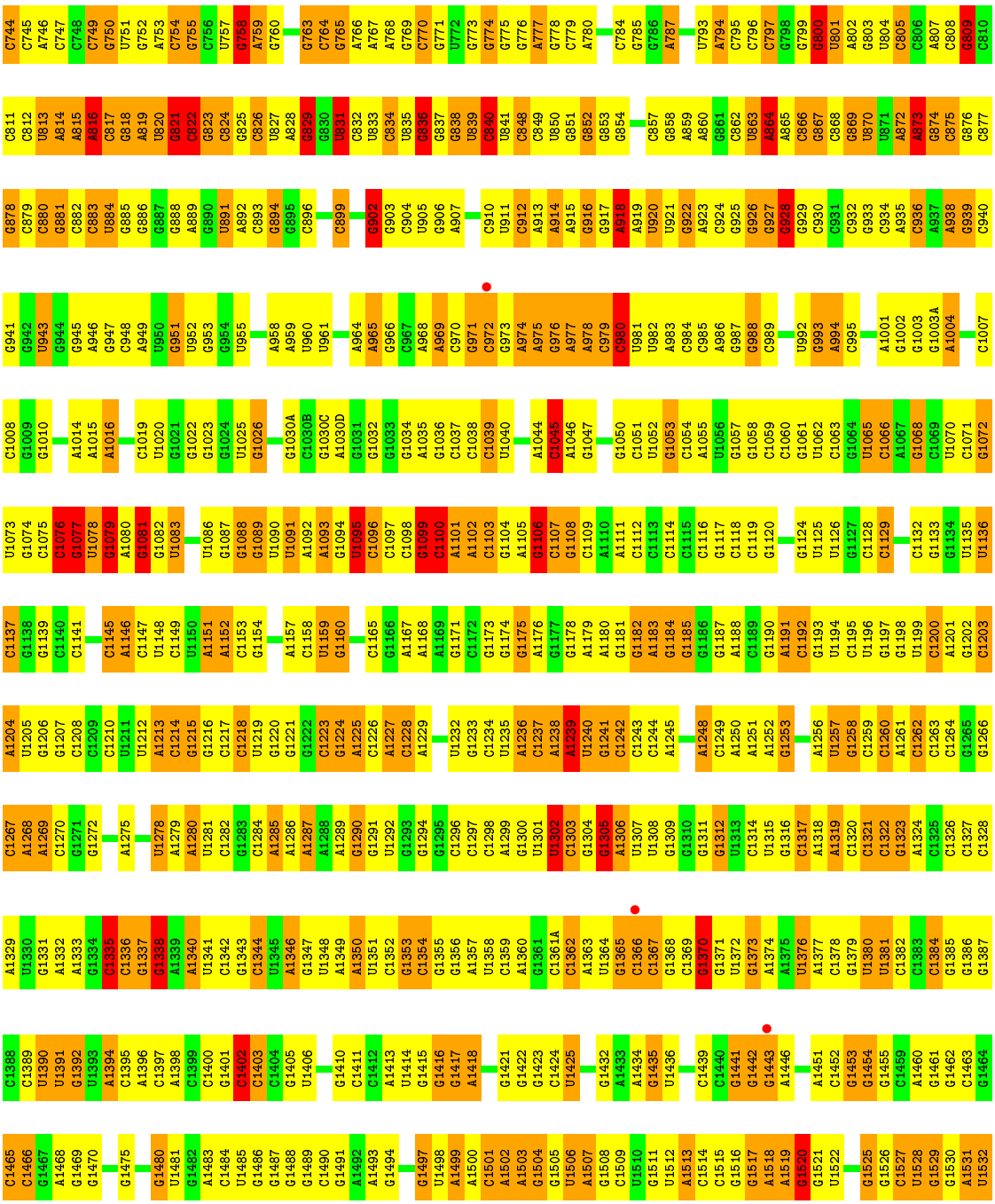
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

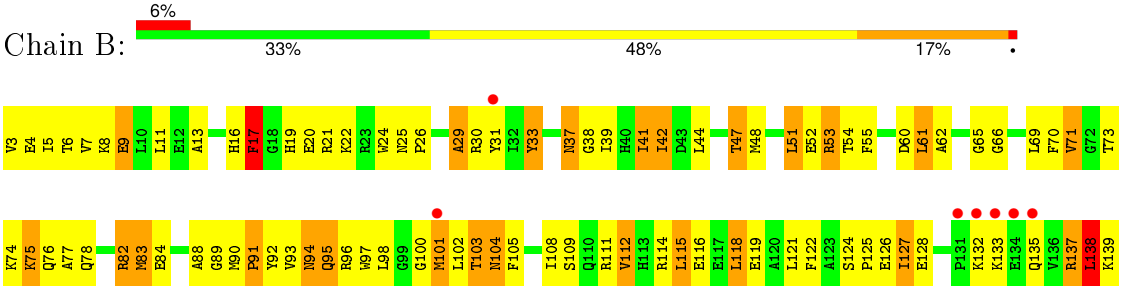
- Molecule 1: 16S ribosomal RNA

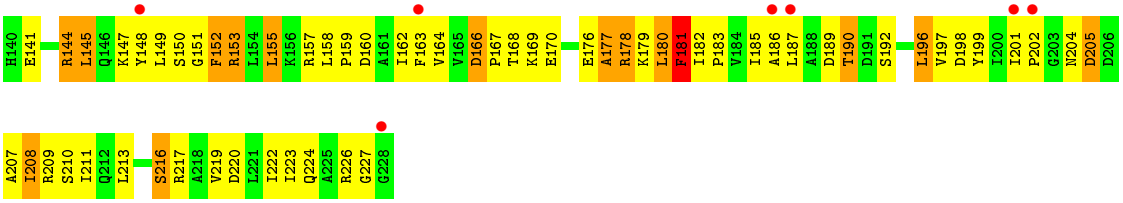
Chain A:



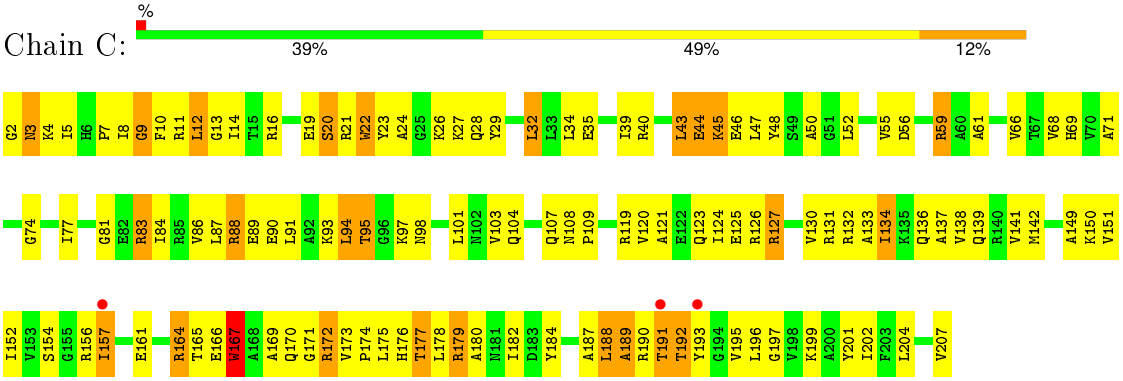


• Molecule 2: 30S ribosomal protein S2

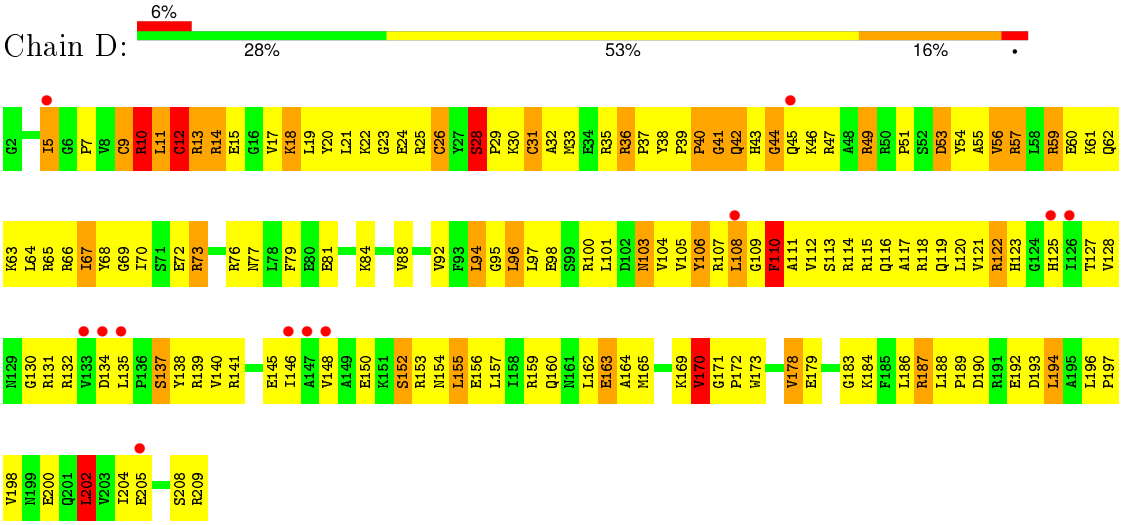




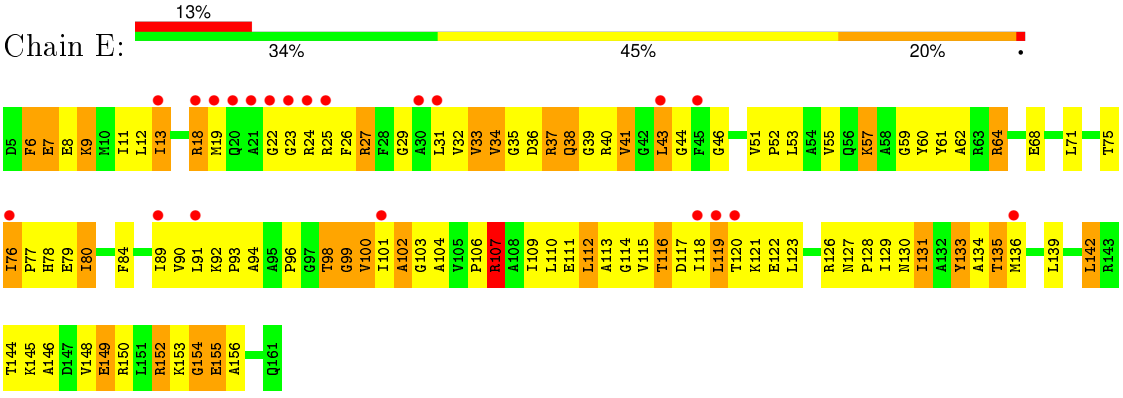
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

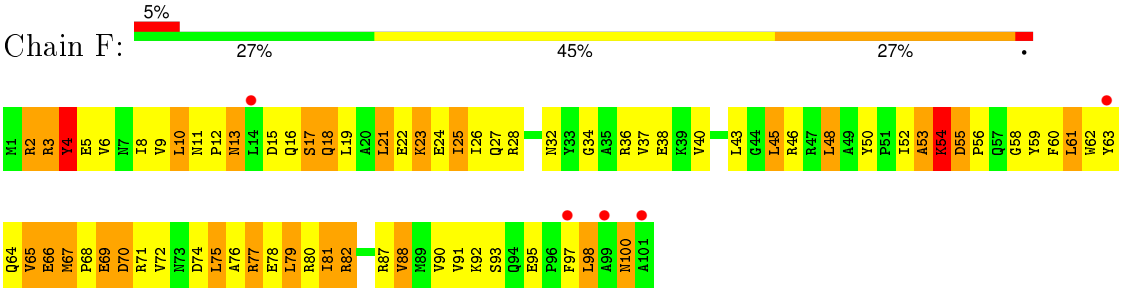


- Molecule 5: 30S ribosomal protein S5



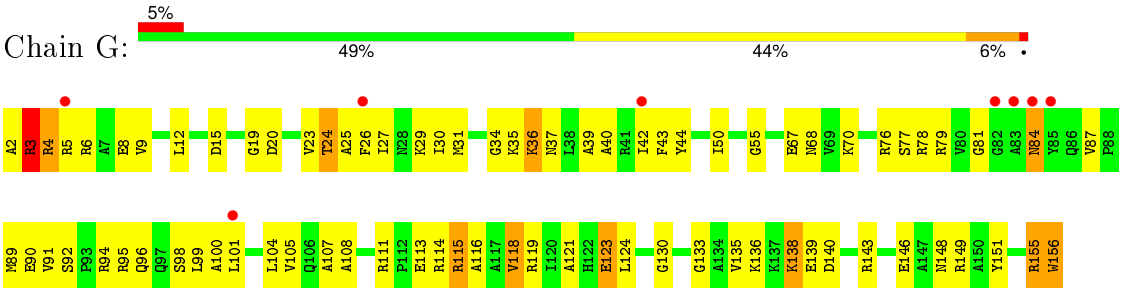
- Molecule 6: 30S ribosomal protein S6

Chain F:



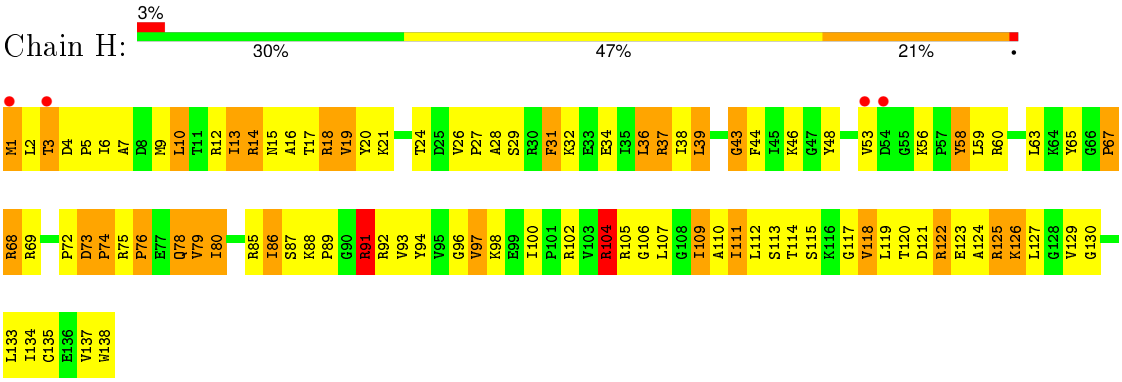
- Molecule 7: 30S ribosomal protein S7

Chain G:



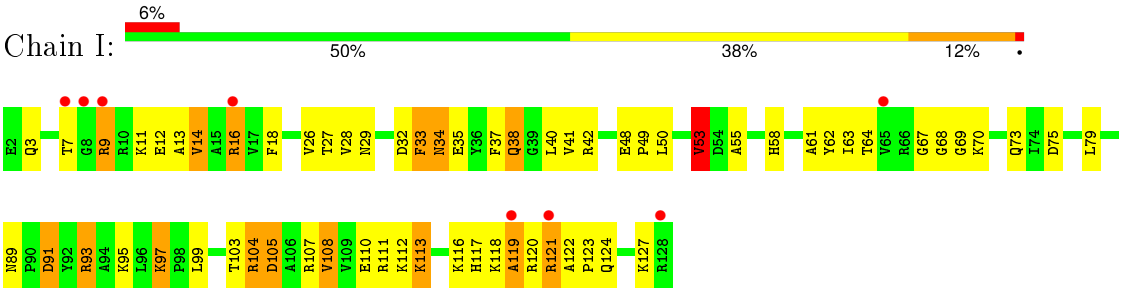
- Molecule 8: 30S ribosomal protein S8

Chain H:



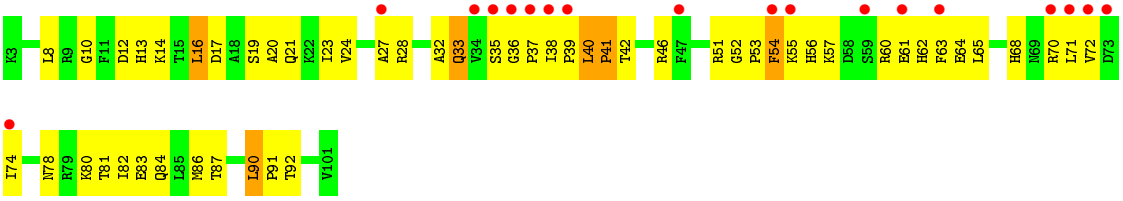
- Molecule 9: 30S ribosomal protein S9

Chain I:



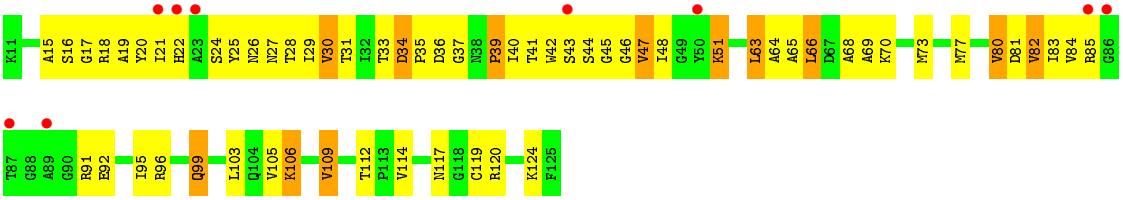
- Molecule 10: 30S ribosomal protein S10

Chain J:



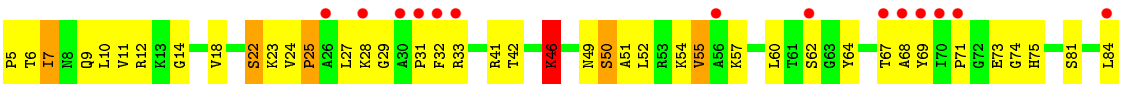
• Molecule 11: 30S ribosomal protein S11

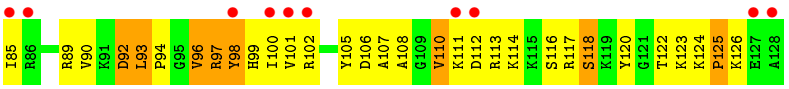
Chain K:



• Molecule 12: 30S ribosomal protein S12

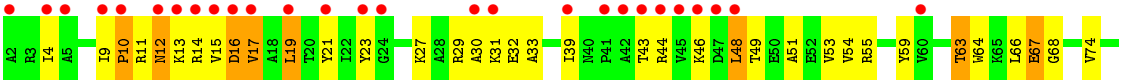
Chain L:

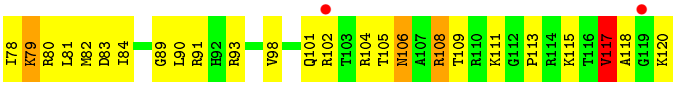




• Molecule 13: 30S ribosomal protein S13

Chain M:



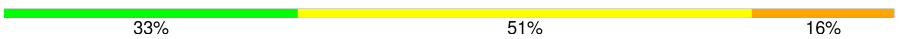


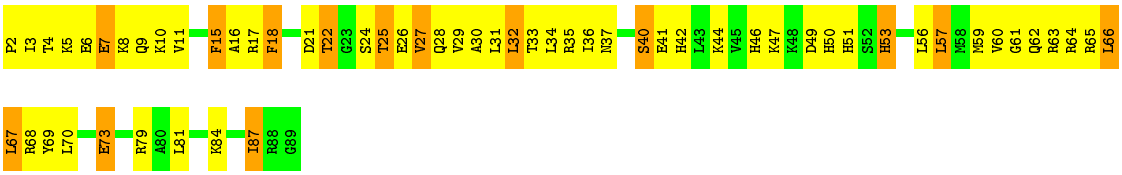
• Molecule 14: 30S ribosomal protein S14 type Z

Chain N:

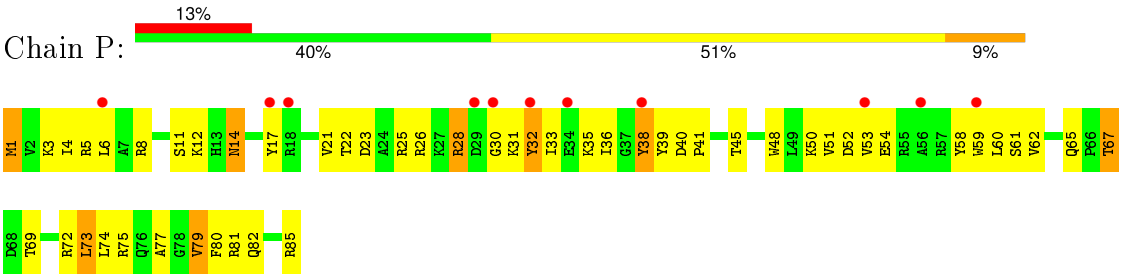
• Molecule 15: 30S ribosomal protein S15

Chain O:

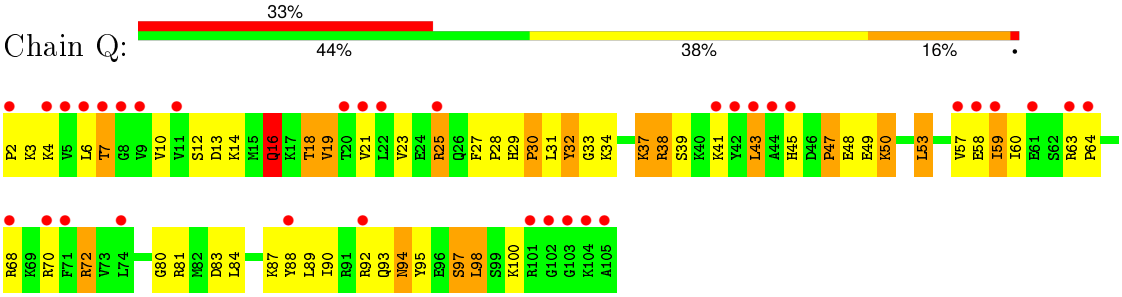




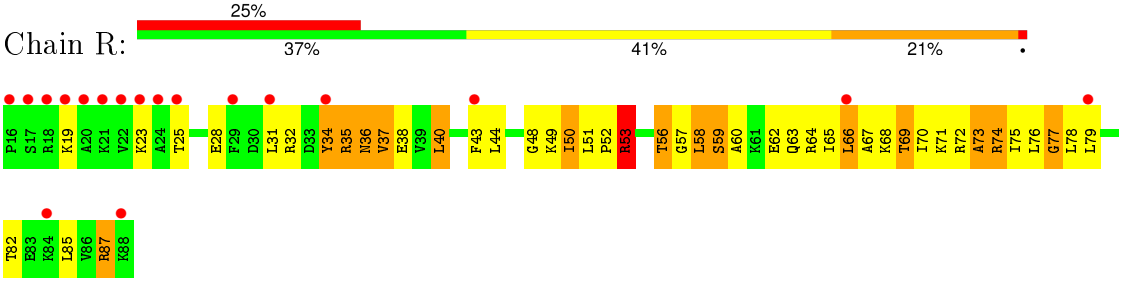
• Molecule 16: 30S ribosomal protein S16



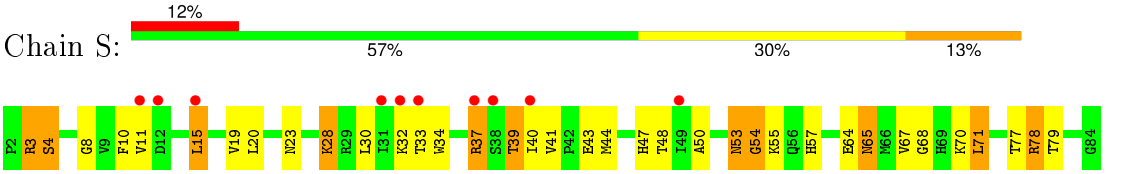
• Molecule 17: 30S ribosomal protein S17



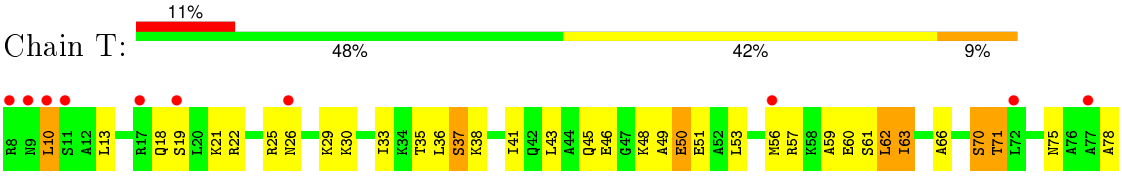
• Molecule 18: 30S ribosomal protein S18



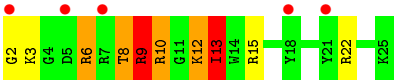
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



• Molecule 21: 30S ribosomal protein Thx



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	409.59Å 409.59Å 171.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 3.42 49.60 – 3.42	Depositor EDS
% Data completeness (in resolution range)	87.5 (48.72-3.42) 87.6 (49.60-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.287 0.230 , 0.285	Depositor DCC
R_{free} test set	8627 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	147.3	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 105.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Outliers	14 of 171522 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	51732	wwPDB-VP
Average B, all atoms (Å^2)	212.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, T1C

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.77	14/36260 (0.0%)	1.43	658/56595 (1.2%)
2	B	0.56	0/1874	0.80	1/2522 (0.0%)
3	C	0.57	0/1637	0.81	0/2205
4	D	0.72	2/1733 (0.1%)	0.94	5/2318 (0.2%)
5	E	0.76	0/1216	1.01	1/1636 (0.1%)
6	F	0.67	0/856	0.94	2/1154 (0.2%)
7	G	0.46	0/1276	0.66	0/1709
8	H	0.74	2/1136 (0.2%)	1.02	3/1527 (0.2%)
9	I	0.47	0/1029	0.67	0/1379
10	J	0.50	0/815	0.73	0/1095
11	K	0.46	0/869	0.68	0/1173
12	L	0.50	0/987	0.78	0/1320
13	M	0.42	0/957	0.67	0/1281
14	N	0.47	0/501	0.79	2/664 (0.3%)
15	O	0.68	2/745 (0.3%)	0.83	0/992
16	P	0.48	0/733	0.75	0/984
17	Q	0.55	0/870	0.80	0/1159
18	R	0.63	0/604	1.04	1/801 (0.1%)
19	S	0.45	0/681	0.63	0/915
20	T	0.44	0/765	0.72	0/1007
21	V	0.51	0/213	0.79	0/277
All	All	0.71	20/55757 (0.0%)	1.27	673/82713 (0.8%)

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
4	D	0	2
6	F	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
17	Q	0	2
All	All	0	7

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	12	CYS	CB-SG	7.79	1.95	1.82
1	A	758	G	N7-C5	-7.24	1.34	1.39
1	A	728	A	N9-C4	6.34	1.41	1.37
1	A	410	G	N9-C4	6.21	1.43	1.38
8	H	123	GLU	CG-CD	6.14	1.61	1.51
1	A	1204	A	N9-C4	5.97	1.41	1.37
15	O	73	GLU	CB-CG	5.90	1.63	1.52
1	A	509	A	N9-C4	5.73	1.41	1.37
8	H	123	GLU	CB-CG	5.71	1.62	1.52
1	A	823	G	N9-C4	5.64	1.42	1.38
4	D	88	VAL	CB-CG2	5.62	1.64	1.52
15	O	73	GLU	CG-CD	5.44	1.60	1.51
1	A	50	A	N9-C4	5.42	1.41	1.37
1	A	702	A	N3-C4	5.42	1.38	1.34
1	A	581	G	C5-C6	-5.41	1.36	1.42
1	A	16	A	N9-C4	5.33	1.41	1.37
1	A	829	G	N7-C5	5.23	1.42	1.39
1	A	1269	A	N9-C4	5.21	1.41	1.37
1	A	124	G	N9-C4	5.17	1.42	1.38
1	A	729	A	N9-C4	5.00	1.40	1.37

All (673) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	578	C	N3-C4-C5	-16.18	115.43	121.90
1	A	578	C	C4-C5-C6	14.72	124.76	117.40
1	A	764	C	C6-N1-C2	-13.75	114.80	120.30
1	A	758	G	C8-N9-C4	-13.19	101.12	106.40
1	A	581	G	N1-C6-O6	13.04	127.72	119.90
1	A	435	C	C6-N1-C2	-11.65	115.64	120.30
1	A	872	A	C4-C5-C6	10.97	122.48	117.00
1	A	758	G	C6-C5-N7	-10.70	123.98	130.40
1	A	917	G	C8-N9-C4	-10.67	102.13	106.40
1	A	823	G	C8-N9-C4	-10.59	102.17	106.40
1	A	1107	C	C6-N1-C2	-10.33	116.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	758	G	N7-C8-N9	10.28	118.24	113.10
1	A	355	C	C6-N1-C2	-10.16	116.23	120.30
1	A	1100	C	N1-C2-O2	10.15	124.99	118.90
1	A	754	C	C2-N3-C4	10.14	124.97	119.90
1	A	237	C	C6-N1-C2	-10.07	116.27	120.30
1	A	571	U	C6-N1-C2	-10.01	115.00	121.00
1	A	764	C	C2-N1-C1'	9.98	129.78	118.80
1	A	764	C	N3-C4-N4	9.95	124.97	118.00
1	A	581	G	C5-C6-O6	-9.80	122.72	128.60
1	A	742	G	N1-C6-O6	-9.78	114.03	119.90
1	A	728	A	N1-C6-N6	-9.78	112.73	118.60
1	A	397	A	N1-C6-N6	-9.75	112.75	118.60
1	A	1096	C	C6-N1-C2	-9.68	116.43	120.30
1	A	433	C	C6-N1-C2	-9.67	116.43	120.30
1	A	18	C	C6-N1-C2	-9.63	116.45	120.30
1	A	764	C	C5-C6-N1	9.60	125.80	121.00
1	A	872	A	N1-C2-N3	9.49	134.04	129.30
1	A	754	C	C2-N1-C1'	9.46	129.21	118.80
1	A	719	C	C6-N1-C2	-9.45	116.52	120.30
1	A	754	C	N1-C2-O2	9.44	124.56	118.90
1	A	824	C	C6-N1-C2	-9.23	116.61	120.30
1	A	1100	C	C2-N1-C1'	9.18	128.90	118.80
1	A	829	G	C8-N9-C4	9.14	110.05	106.40
1	A	717	C	C5-C6-N1	9.11	125.56	121.00
1	A	882	C	C6-N1-C2	9.04	123.92	120.30
1	A	110	C	C6-N1-C2	-9.02	116.69	120.30
1	A	989	C	C6-N1-C2	-8.99	116.70	120.30
1	A	311	C	N3-C2-O2	-8.95	115.64	121.90
1	A	578	C	C6-N1-C2	-8.95	116.72	120.30
1	A	1077	G	C8-N9-C4	-8.91	102.84	106.40
1	A	174	C	C6-N1-C2	-8.88	116.75	120.30
1	A	667	G	C5-C6-O6	-8.84	123.30	128.60
1	A	683	G	C8-N9-C4	-8.82	102.87	106.40
1	A	410	G	N3-C4-C5	-8.79	124.20	128.60
1	A	980	C	C6-N1-C2	-8.78	116.79	120.30
1	A	765	G	C4-C5-N7	-8.78	107.29	110.80
1	A	755	G	C8-N9-C4	-8.77	102.89	106.40
1	A	581	G	C4-C5-N7	8.76	114.31	110.80
1	A	503	C	C6-N1-C2	-8.72	116.81	120.30
1	A	73	C	C6-N1-C2	-8.71	116.81	120.30
1	A	37	U	C5-C6-N1	8.71	127.05	122.70
1	A	1108	G	N1-C6-O6	-8.59	114.75	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	557	G	C4-N9-C1'	8.58	137.66	126.50
1	A	486	U	C2-N1-C1'	8.57	127.98	117.70
1	A	298	A	C4-C5-C6	8.57	121.28	117.00
1	A	1078	U	N3-C2-O2	-8.56	116.21	122.20
1	A	311	C	N1-C2-O2	8.53	124.02	118.90
1	A	1158	C	C2-N1-C1'	8.51	128.16	118.80
1	A	1501	C	C6-N1-C2	-8.50	116.90	120.30
1	A	824	C	C2-N1-C1'	8.47	128.12	118.80
1	A	965	A	C8-N9-C4	8.46	109.18	105.80
1	A	873	A	N1-C6-N6	-8.42	113.55	118.60
1	A	1089	G	C8-N9-C4	-8.40	103.04	106.40
1	A	734	G	C8-N9-C4	-8.35	103.06	106.40
1	A	823	G	N7-C8-N9	8.34	117.27	113.10
1	A	930	C	C6-N1-C2	-8.33	116.97	120.30
1	A	110	C	C2-N1-C1'	8.31	127.95	118.80
1	A	755	G	C4-N9-C1'	8.30	137.30	126.50
1	A	1158	C	N1-C2-O2	8.27	123.86	118.90
1	A	1526	G	C8-N9-C4	-8.23	103.11	106.40
1	A	407	G	C8-N9-C4	-8.22	103.11	106.40
1	A	557	G	N3-C4-C5	-8.20	124.50	128.60
1	A	1093	A	C4-C5-C6	8.18	121.09	117.00
1	A	1465	C	C6-N1-C2	-8.14	117.04	120.30
1	A	717	C	N3-C4-N4	8.13	123.69	118.00
1	A	928	G	C8-N9-C4	-8.13	103.15	106.40
1	A	765	G	N9-C4-C5	8.12	108.65	105.40
1	A	758	G	N1-C6-O6	8.12	124.77	119.90
1	A	516	U	C6-N1-C2	-8.11	116.14	121.00
1	A	634	C	C6-N1-C2	-8.10	117.06	120.30
1	A	294	U	C6-N1-C2	-8.10	116.14	121.00
1	A	744	C	C5-C6-N1	8.09	125.04	121.00
1	A	660	G	C8-N9-C4	-8.04	103.19	106.40
1	A	667	G	C4-C5-N7	8.00	114.00	110.80
1	A	836	G	N1-C6-O6	7.99	124.69	119.90
1	A	578	C	N3-C4-N4	7.96	123.57	118.00
1	A	667	G	N1-C6-O6	7.96	124.67	119.90
1	A	754	C	N3-C4-C5	-7.95	118.72	121.90
1	A	881	G	N3-C4-N9	-7.95	121.23	126.00
1	A	881	G	C4-N9-C1'	-7.94	116.17	126.50
1	A	40	C	C6-N1-C2	-7.92	117.13	120.30
1	A	881	G	N3-C4-C5	7.89	132.55	128.60
1	A	834	C	C5-C6-N1	7.89	124.94	121.00
1	A	373	A	C8-N9-C4	7.84	108.94	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	878	G	N3-C4-N9	7.83	130.70	126.00
1	A	563	A	N1-C6-N6	7.82	123.29	118.60
1	A	854	G	N1-C6-O6	7.82	124.59	119.90
1	A	564	C	C5-C6-N1	7.81	124.91	121.00
1	A	298	A	C8-N9-C4	-7.80	102.68	105.80
1	A	730	G	C8-N9-C4	-7.77	103.29	106.40
1	A	663	A	N1-C6-N6	-7.74	113.95	118.60
1	A	824	C	N3-C4-N4	7.73	123.41	118.00
1	A	872	A	C4-N9-C1'	7.71	140.19	126.30
1	A	881	G	C8-N9-C1'	7.71	137.03	127.00
1	A	824	C	C5-C6-N1	7.69	124.84	121.00
1	A	874	G	N1-C6-O6	7.68	124.51	119.90
1	A	1095	U	C5-C6-N1	7.67	126.53	122.70
1	A	733	A	C8-N9-C4	7.66	108.86	105.80
1	A	829	G	N7-C8-N9	-7.65	109.27	113.10
1	A	1114	C	C5-C6-N1	7.63	124.82	121.00
1	A	615	C	C5-C6-N1	7.63	124.81	121.00
1	A	1096	C	C5-C6-N1	7.62	124.81	121.00
1	A	769	G	C8-N9-C4	7.60	109.44	106.40
1	A	721	G	C4-N9-C1'	7.59	136.37	126.50
1	A	427	U	C2-N1-C1'	7.57	126.79	117.70
1	A	754	C	C6-N1-C1'	-7.55	111.74	120.80
1	A	295	C	C5-C6-N1	7.55	124.77	121.00
1	A	581	G	C6-C5-N7	-7.55	125.87	130.40
1	A	435	C	C5-C6-N1	7.54	124.77	121.00
1	A	1114	C	C6-N1-C2	-7.52	117.29	120.30
1	A	800	G	C8-N9-C4	-7.51	103.40	106.40
1	A	742	G	C5-C6-O6	7.50	133.10	128.60
1	A	1078	U	N1-C2-O2	7.48	128.04	122.80
1	A	124	G	N3-C4-C5	-7.47	124.86	128.60
1	A	503	C	N3-C2-O2	-7.47	116.67	121.90
1	A	545	C	N1-C2-O2	7.47	123.38	118.90
1	A	671	G	C8-N9-C4	-7.45	103.42	106.40
1	A	912	C	N3-C4-C5	-7.44	118.92	121.90
1	A	564	C	C2-N3-C4	7.42	123.61	119.90
1	A	595	G	C8-N9-C4	-7.41	103.44	106.40
1	A	1529	G	N3-C4-N9	7.40	130.44	126.00
1	A	509	A	C5-N7-C8	7.40	107.60	103.90
1	A	540	G	C8-N9-C4	-7.37	103.45	106.40
1	A	1204	A	C8-N9-C4	-7.36	102.86	105.80
1	A	1077	G	N3-C4-C5	-7.35	124.93	128.60
1	A	18	C	N3-C4-C5	-7.34	118.96	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1185	G	C8-N9-C4	-7.34	103.47	106.40
1	A	1192	C	C6-N1-C2	-7.33	117.37	120.30
1	A	571	U	C5-C6-N1	7.33	126.37	122.70
1	A	410	G	C4-N9-C1'	7.32	136.02	126.50
1	A	457	C	C6-N1-C2	-7.32	117.37	120.30
1	A	572	A	N1-C6-N6	-7.32	114.21	118.60
1	A	1335	C	N1-C2-O2	7.30	123.28	118.90
1	A	1382	C	C6-N1-C2	7.29	123.22	120.30
1	A	729	A	C8-N9-C4	-7.29	102.89	105.80
1	A	366	C	C6-N1-C2	-7.28	117.39	120.30
1	A	918	A	C8-N9-C4	-7.27	102.89	105.80
1	A	442	C	C6-N1-C2	-7.27	117.39	120.30
1	A	366	C	N3-C4-C5	-7.27	118.99	121.90
1	A	410	G	C8-N9-C4	-7.26	103.50	106.40
1	A	872	A	N3-C4-C5	-7.26	121.72	126.80
1	A	728	A	C8-N9-C4	-7.25	102.90	105.80
1	A	819	A	N1-C6-N6	7.24	122.95	118.60
1	A	672	U	N3-C4-O4	7.24	124.47	119.40
1	A	912	C	C6-N1-C2	-7.21	117.41	120.30
1	A	834	C	C4-C5-C6	-7.21	113.80	117.40
1	A	1526	G	C4-C5-C6	7.19	123.11	118.80
1	A	649	G	N1-C6-O6	7.17	124.20	119.90
1	A	241	C	C6-N1-C2	7.15	123.16	120.30
1	A	717	C	C5-C4-N4	-7.15	115.20	120.20
1	A	659	U	C6-N1-C2	-7.14	116.72	121.00
1	A	551	U	C2-N1-C1'	-7.12	109.16	117.70
1	A	717	C	C6-N1-C2	-7.12	117.45	120.30
1	A	728	A	N9-C4-C5	7.10	108.64	105.80
1	A	488	C	C6-N1-C2	-7.10	117.46	120.30
1	A	1045	C	C6-N1-C2	-7.05	117.48	120.30
1	A	568	G	N3-C2-N2	-7.05	114.97	119.90
1	A	563	A	C2-N3-C4	-7.01	107.09	110.60
1	A	1100	C	N3-C2-O2	-7.01	116.99	121.90
1	A	571	U	N3-C2-O2	-6.99	117.31	122.20
1	A	739	C	C5-C6-N1	6.97	124.49	121.00
1	A	295	C	C6-N1-C2	-6.96	117.51	120.30
1	A	1529	G	C8-N9-C1'	-6.95	117.96	127.00
1	A	980	C	C6-N1-C1'	6.95	129.14	120.80
1	A	294	U	C5-C6-N1	6.94	126.17	122.70
1	A	1108	G	C8-N9-C4	-6.93	103.63	106.40
1	A	563	A	N9-C4-C5	-6.93	103.03	105.80
1	A	1077	G	C6-C5-N7	-6.93	126.25	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1532	U	C5-C6-N1	6.93	126.16	122.70
1	A	1338	G	N3-C4-C5	-6.92	125.14	128.60
1	A	872	A	C6-C5-N7	-6.90	127.47	132.30
1	A	150	C	C6-N1-C2	-6.90	117.54	120.30
5	E	107	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	728	A	C2-N3-C4	6.87	114.04	110.60
1	A	1529	G	C4-N9-C1'	6.87	135.43	126.50
1	A	1107	C	C5-C6-N1	6.86	124.43	121.00
1	A	916	G	C8-N9-C4	-6.84	103.67	106.40
1	A	366	C	C4-C5-C6	6.83	120.81	117.40
1	A	980	C	N3-C2-O2	-6.83	117.12	121.90
1	A	755	G	C6-C5-N7	-6.82	126.31	130.40
1	A	510	A	C5-C6-N1	6.81	121.10	117.70
1	A	586	C	C6-N1-C2	-6.80	117.58	120.30
1	A	581	G	C5-N7-C8	-6.80	100.90	104.30
1	A	872	A	C6-N1-C2	-6.80	114.52	118.60
1	A	426	G	N3-C4-N9	6.79	130.07	126.00
1	A	242	C	C2-N1-C1'	-6.78	111.35	118.80
1	A	99	C	C6-N1-C2	-6.77	117.59	120.30
1	A	574	A	C8-N9-C4	6.77	108.51	105.80
1	A	873	A	N9-C4-C5	6.77	108.51	105.80
1	A	809	G	C8-N9-C4	6.77	109.11	106.40
1	A	1501	C	N3-C4-C5	-6.77	119.19	121.90
1	A	1095	U	C6-N1-C2	-6.77	116.94	121.00
1	A	917	G	N7-C8-N9	6.77	116.48	113.10
1	A	397	A	C2-N3-C4	6.75	113.97	110.60
1	A	557	G	N3-C4-N9	6.75	130.05	126.00
1	A	563	A	C5-N7-C8	-6.75	100.53	103.90
4	D	12	CYS	CA-CB-SG	6.75	126.15	114.00
1	A	755	G	N7-C8-N9	6.74	116.47	113.10
1	A	504	C	C5-C6-N1	6.73	124.36	121.00
1	A	684	A	C8-N9-C4	-6.72	103.11	105.80
1	A	764	C	N3-C4-C5	-6.70	119.22	121.90
1	A	433	C	C5-C6-N1	6.70	124.35	121.00
1	A	742	G	C4-C5-N7	-6.70	108.12	110.80
1	A	278	G	C8-N9-C4	-6.70	103.72	106.40
1	A	1158	C	C6-N1-C1'	-6.69	112.77	120.80
1	A	177	C	N1-C2-O2	6.68	122.91	118.90
1	A	765	G	C5-C6-O6	6.68	132.61	128.60
1	A	557	G	C8-N9-C1'	-6.67	118.33	127.00
1	A	721	G	C8-N9-C1'	-6.67	118.33	127.00
1	A	110	C	N3-C2-O2	-6.66	117.24	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1403	C	C6-N1-C2	-6.66	117.64	120.30
1	A	730	G	N3-C4-C5	-6.65	125.28	128.60
1	A	965	A	N7-C8-N9	-6.64	110.48	113.80
1	A	1302	U	N1-C2-O2	6.64	127.44	122.80
1	A	926	G	N3-C4-N9	6.63	129.98	126.00
1	A	743	U	N1-C2-O2	6.62	127.43	122.80
1	A	224	C	C6-N1-C2	-6.62	117.65	120.30
1	A	1453	G	N3-C4-N9	6.61	129.97	126.00
1	A	298	A	N1-C2-N3	6.61	132.60	129.30
1	A	1100	C	C6-N1-C1'	-6.59	112.89	120.80
1	A	758	G	C4-C5-N7	6.58	113.43	110.80
1	A	742	G	N9-C4-C5	6.58	108.03	105.40
1	A	323	U	C5-C6-N1	6.57	125.99	122.70
1	A	811	C	N3-C2-O2	-6.57	117.30	121.90
1	A	486	U	C6-N1-C1'	-6.57	112.01	121.20
1	A	743	U	N3-C2-O2	-6.56	117.61	122.20
1	A	410	G	C4-C5-C6	6.56	122.73	118.80
1	A	1402	C	C6-N1-C2	-6.56	117.68	120.30
1	A	1302	U	C2-N1-C1'	6.55	125.56	117.70
1	A	298	A	N7-C8-N9	6.54	117.07	113.80
1	A	755	G	C4-C5-C6	6.53	122.72	118.80
1	A	654	G	N9-C4-C5	-6.52	102.79	105.40
1	A	1089	G	N7-C8-N9	6.52	116.36	113.10
1	A	734	G	N7-C8-N9	6.51	116.36	113.10
1	A	615	C	C6-N1-C2	-6.51	117.70	120.30
1	A	400	C	C6-N1-C2	-6.51	117.70	120.30
1	A	717	C	C2-N1-C1'	6.50	125.95	118.80
1	A	1384	C	C6-N1-C2	-6.50	117.70	120.30
1	A	372	C	C6-N1-C2	6.50	122.90	120.30
1	A	863	U	N3-C2-O2	-6.50	117.65	122.20
1	A	994	A	C8-N9-C4	-6.49	103.20	105.80
1	A	618	C	C6-N1-C2	-6.48	117.71	120.30
1	A	809	G	N9-C4-C5	-6.48	102.81	105.40
1	A	1509	C	C6-N1-C2	-6.46	117.72	120.30
1	A	435	C	C2-N1-C1'	6.45	125.90	118.80
1	A	809	G	N1-C6-O6	6.45	123.77	119.90
18	R	53	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	1401	G	C8-N9-C4	-6.45	103.82	106.40
1	A	754	C	C5-C6-N1	6.45	124.22	121.00
1	A	366	C	C5-C4-N4	6.44	124.71	120.20
1	A	1232	U	C6-N1-C2	-6.44	117.14	121.00
1	A	816	A	N9-C4-C5	6.43	108.37	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1168	A	C8-N9-C4	-6.43	103.23	105.80
1	A	557	G	C8-N9-C4	-6.42	103.83	106.40
1	A	832	C	C6-N1-C2	6.42	122.87	120.30
1	A	891	U	C6-N1-C2	-6.41	117.15	121.00
1	A	8	A	C8-N9-C4	-6.41	103.24	105.80
1	A	385	C	C6-N1-C2	-6.41	117.74	120.30
1	A	1285	A	C8-N9-C4	6.40	108.36	105.80
1	A	124	G	C8-N9-C4	-6.40	103.84	106.40
1	A	19	C	N3-C2-O2	-6.39	117.43	121.90
1	A	899	C	N1-C2-O2	6.39	122.73	118.90
1	A	1453	G	N3-C4-C5	-6.39	125.41	128.60
1	A	1373	G	N3-C4-C5	-6.39	125.41	128.60
1	A	1108	G	C5-C6-O6	6.38	132.43	128.60
1	A	434	U	C5-C6-N1	6.37	125.88	122.70
1	A	459	G	N1-C6-O6	6.36	123.72	119.90
1	A	971	G	C4-C5-N7	-6.36	108.26	110.80
1	A	1381	U	N1-C2-O2	6.35	127.25	122.80
1	A	848	C	C6-N1-C2	-6.34	117.76	120.30
1	A	115	G	N9-C4-C5	-6.33	102.87	105.40
1	A	564	C	C6-N1-C2	-6.33	117.77	120.30
1	A	875	C	C6-N1-C2	-6.33	117.77	120.30
1	A	918	A	N7-C8-N9	6.32	116.96	113.80
1	A	488	C	C5-C6-N1	6.31	124.16	121.00
1	A	980	C	N1-C2-N3	6.30	123.61	119.20
1	A	683	G	N7-C8-N9	6.30	116.25	113.10
1	A	758	G	C4-C5-C6	6.29	122.58	118.80
1	A	623	C	C5-C6-N1	6.29	124.14	121.00
1	A	823	G	N3-C4-C5	-6.28	125.46	128.60
1	A	1335	C	N3-C2-O2	-6.28	117.50	121.90
1	A	764	C	C5-C4-N4	-6.28	115.81	120.20
1	A	872	A	C8-N9-C1'	-6.27	116.41	127.70
1	A	816	A	C5-C6-N6	6.27	128.72	123.70
1	A	40	C	N3-C2-O2	-6.27	117.51	121.90
1	A	1453	G	C4-N9-C1'	6.26	134.65	126.50
1	A	874	G	C4-C5-N7	6.26	113.30	110.80
1	A	300	A	N1-C6-N6	-6.25	114.85	118.60
1	A	717	C	C2-N3-C4	6.25	123.03	119.90
1	A	1529	G	N3-C4-C5	-6.25	125.47	128.60
1	A	295	C	N3-C4-N4	6.25	122.37	118.00
1	A	40	C	C2-N1-C1'	6.24	125.67	118.80
1	A	1096	C	N3-C4-C5	-6.23	119.41	121.90
1	A	1192	C	C2-N1-C1'	6.22	125.64	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	821	G	N1-C6-O6	-6.22	116.17	119.90
1	A	545	C	N3-C2-O2	-6.21	117.55	121.90
1	A	1338	G	N3-C4-N9	6.21	129.73	126.00
1	A	824	C	N1-C2-O2	6.20	122.62	118.90
1	A	916	G	N3-C4-C5	-6.20	125.50	128.60
1	A	1392	G	C8-N9-C4	-6.20	103.92	106.40
1	A	1340	A	C8-N9-C4	-6.19	103.32	105.80
1	A	388	G	C6-C5-N7	6.18	134.11	130.40
1	A	672	U	C5-C6-N1	6.17	125.79	122.70
1	A	1526	G	C4-N9-C1'	6.17	134.53	126.50
1	A	547	A	N9-C4-C5	6.17	108.27	105.80
1	A	1507	A	C8-N9-C4	-6.17	103.33	105.80
1	A	406	G	C4-N9-C1'	6.17	134.51	126.50
1	A	1384	C	C5-C6-N1	6.16	124.08	121.00
1	A	328	C	C2-N1-C1'	-6.15	112.03	118.80
1	A	1205	U	N3-C2-O2	-6.15	117.89	122.20
1	A	1504	G	C8-N9-C4	-6.14	103.94	106.40
1	A	298	A	C6-C5-N7	-6.14	128.00	132.30
1	A	926	G	N3-C2-N2	6.12	124.19	119.90
1	A	765	G	N3-C2-N2	-6.12	115.61	119.90
1	A	872	A	N3-C4-N9	6.12	132.29	127.40
1	A	924	C	C6-N1-C1'	6.12	128.14	120.80
1	A	1103	C	N1-C2-O2	6.12	122.57	118.90
1	A	505	G	C4-N9-C1'	6.11	134.44	126.50
1	A	46	G	C8-N9-C4	-6.08	103.97	106.40
1	A	672	U	C6-N1-C2	-6.07	117.36	121.00
1	A	765	G	C5-C6-N1	-6.07	108.47	111.50
1	A	878	G	N3-C4-C5	-6.06	125.57	128.60
1	A	829	G	C6-C5-N7	6.06	134.04	130.40
1	A	1100	C	C5-C6-N1	6.06	124.03	121.00
1	A	17	U	C6-N1-C2	-6.06	117.36	121.00
1	A	547	A	N1-C6-N6	-6.06	114.97	118.60
1	A	1526	G	C6-C5-N7	-6.05	126.77	130.40
1	A	562	C	N1-C2-O2	6.05	122.53	118.90
1	A	551	U	C5-C6-N1	-6.05	119.68	122.70
1	A	755	G	N3-C4-C5	-6.04	125.58	128.60
1	A	296	U	N3-C4-C5	-6.04	110.98	114.60
1	A	938	A	C8-N9-C4	-6.04	103.39	105.80
1	A	442	C	C5-C6-N1	6.03	124.02	121.00
1	A	949	A	C8-N9-C4	-6.01	103.40	105.80
1	A	1223	C	N3-C2-O2	-6.01	117.69	121.90
1	A	654	G	C4-C5-N7	6.00	113.20	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	758	G	C4-N9-C1'	6.00	134.31	126.50
1	A	872	A	C8-N9-C4	-6.00	103.40	105.80
1	A	819	A	C4-C5-N7	5.99	113.70	110.70
1	A	1081	G	C4-N9-C1'	-5.99	118.72	126.50
1	A	684	A	N7-C8-N9	5.98	116.79	113.80
1	A	866	C	N3-C2-O2	-5.98	117.71	121.90
1	A	509	A	C4-C5-N7	-5.98	107.71	110.70
1	A	586	C	C5-C6-N1	5.98	123.99	121.00
1	A	22	G	C2-N3-C4	-5.98	108.91	111.90
1	A	397	A	C5-C6-N1	5.97	120.68	117.70
1	A	840	C	N1-C2-O2	5.97	122.48	118.90
1	A	874	G	C5-C6-O6	-5.97	125.02	128.60
1	A	819	A	N9-C4-C5	-5.96	103.41	105.80
1	A	174	C	C5-C6-N1	5.95	123.98	121.00
1	A	1165	C	C6-N1-C2	-5.95	117.92	120.30
1	A	929	G	N1-C6-O6	5.95	123.47	119.90
1	A	936	C	C6-N1-C2	-5.94	117.92	120.30
1	A	503	C	N1-C2-O2	5.93	122.45	118.90
1	A	362	G	C8-N9-C4	-5.91	104.04	106.40
1	A	825	G	N3-C4-N9	5.91	129.54	126.00
1	A	566	G	C4-C5-N7	-5.90	108.44	110.80
1	A	733	A	N7-C8-N9	-5.90	110.85	113.80
1	A	237	C	C5-C6-N1	5.89	123.94	121.00
1	A	1526	G	N7-C8-N9	5.89	116.05	113.10
1	A	1436	U	C5-C6-N1	5.89	125.64	122.70
1	A	829	G	C4-N9-C1'	-5.88	118.85	126.50
1	A	362	G	N7-C8-N9	5.88	116.04	113.10
1	A	481	G	N3-C4-C5	-5.88	125.66	128.60
1	A	1501	C	N3-C2-O2	-5.88	117.78	121.90
1	A	578	C	C2-N1-C1'	5.88	125.26	118.80
1	A	34	C	N3-C4-C5	-5.88	119.55	121.90
1	A	1381	U	N3-C2-O2	-5.87	118.09	122.20
1	A	260	G	C8-N9-C4	-5.87	104.05	106.40
1	A	551	U	N3-C4-O4	-5.86	115.30	119.40
1	A	1344	C	N1-C2-O2	5.86	122.42	118.90
1	A	750	G	N3-C4-N9	5.86	129.51	126.00
1	A	1079	G	N1-C6-O6	5.84	123.41	119.90
1	A	1077	G	C4-C5-C6	5.82	122.29	118.80
1	A	1242	C	C5-C6-N1	5.82	123.91	121.00
1	A	40	C	N1-C2-O2	5.80	122.38	118.90
1	A	296	U	N3-C4-O4	5.80	123.46	119.40
1	A	509	A	N1-C6-N6	-5.80	115.12	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	740	U	N1-C2-O2	-5.79	118.74	122.80
1	A	864	A	N1-C6-N6	-5.79	115.13	118.60
1	A	740	U	C2-N1-C1'	-5.78	110.76	117.70
1	A	553	A	C8-N9-C4	5.78	108.11	105.80
1	A	725	G	N9-C4-C5	-5.76	103.10	105.40
1	A	831	U	N1-C2-O2	5.76	126.83	122.80
1	A	486	U	N1-C2-O2	5.75	126.83	122.80
1	A	516	U	N3-C2-O2	-5.75	118.17	122.20
1	A	55	A	C8-N9-C4	-5.75	103.50	105.80
1	A	750	G	N3-C4-C5	-5.74	125.73	128.60
2	B	138	LEU	CA-CB-CG	5.74	128.51	115.30
1	A	1072	G	N3-C4-N9	5.74	129.44	126.00
1	A	124	G	N3-C4-N9	5.74	129.44	126.00
1	A	732	C	N3-C2-O2	-5.73	117.89	121.90
1	A	505	G	C8-N9-C4	-5.72	104.11	106.40
1	A	561	U	C5-C6-N1	5.72	125.56	122.70
1	A	692	U	C5-C6-N1	5.72	125.56	122.70
1	A	719	C	C5-C6-N1	5.72	123.86	121.00
1	A	920	U	C5-C4-O4	5.72	129.33	125.90
1	A	758	G	C5-C6-O6	-5.72	125.17	128.60
1	A	836	G	C8-N9-C4	-5.72	104.11	106.40
1	A	1390	U	N3-C4-O4	-5.71	115.40	119.40
1	A	563	A	C5-C6-N1	-5.71	114.85	117.70
1	A	1135	U	C6-N1-C2	-5.70	117.58	121.00
1	A	725	G	C6-C5-N7	-5.70	126.98	130.40
1	A	1203	C	C6-N1-C2	-5.70	118.02	120.30
1	A	1191	A	C8-N9-C4	-5.70	103.52	105.80
1	A	410	G	N3-C4-N9	5.70	129.42	126.00
1	A	863	U	C4-C5-C6	5.69	123.11	119.70
1	A	1108	G	N3-C4-C5	-5.69	125.75	128.60
1	A	902	G	C4-N9-C1'	-5.69	119.10	126.50
1	A	115	G	C8-N9-C4	5.68	108.67	106.40
1	A	435	C	N3-C2-O2	-5.68	117.93	121.90
1	A	1093	A	N3-C4-C5	-5.66	122.84	126.80
1	A	873	A	C5-C6-N6	5.66	128.22	123.70
1	A	1305	G	N3-C2-N2	-5.65	115.94	119.90
1	A	739	C	C4-C5-C6	-5.65	114.58	117.40
1	A	1091	U	N3-C2-O2	-5.65	118.25	122.20
1	A	595	G	N3-C4-C5	-5.64	125.78	128.60
1	A	824	C	C5-C4-N4	-5.64	116.25	120.20
1	A	28	G	C8-N9-C4	-5.64	104.14	106.40
1	A	328	C	C6-N1-C1'	5.63	127.56	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	505	G	N3-C4-C5	-5.63	125.78	128.60
1	A	758	G	C5-N7-C8	-5.63	101.48	104.30
1	A	784	C	C6-N1-C2	5.63	122.55	120.30
1	A	1215	G	C4-N9-C1'	5.62	133.81	126.50
1	A	774	G	C8-N9-C4	-5.62	104.15	106.40
1	A	1340	A	N7-C8-N9	5.62	116.61	113.80
1	A	654	G	C5-C6-O6	-5.62	125.23	128.60
1	A	744	C	C6-N1-C2	-5.62	118.05	120.30
1	A	20	U	N3-C2-O2	5.61	126.13	122.20
1	A	1370	G	C8-N9-C4	-5.61	104.16	106.40
1	A	1072	G	N3-C4-C5	-5.60	125.80	128.60
1	A	1076	C	C5-C6-N1	5.60	123.80	121.00
1	A	770	C	N3-C4-C5	5.60	124.14	121.90
1	A	881	G	N3-C2-N2	-5.60	115.98	119.90
1	A	623	C	C6-N1-C2	-5.59	118.06	120.30
1	A	1403	C	C2-N1-C1'	5.59	124.95	118.80
1	A	1099	G	C8-N9-C4	-5.58	104.17	106.40
1	A	1100	C	C6-N1-C2	-5.58	118.07	120.30
1	A	1526	G	C5-C6-N1	-5.58	108.71	111.50
1	A	740	U	N3-C2-O2	5.57	126.10	122.20
6	F	4	TYR	N-CA-C	5.56	126.02	111.00
1	A	93	G	C8-N9-C4	5.56	108.62	106.40
14	N	44	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	540	G	N7-C8-N9	5.55	115.88	113.10
1	A	1453	G	C8-N9-C1'	-5.55	119.78	127.00
1	A	667	G	C5-N7-C8	-5.55	101.52	104.30
1	A	867	G	C5-C6-O6	-5.55	125.27	128.60
1	A	755	G	C8-N9-C1'	-5.55	119.78	127.00
1	A	384	G	C6-C5-N7	-5.55	127.07	130.40
1	A	839	U	C2-N1-C1'	5.55	124.36	117.70
1	A	1435	G	N1-C6-O6	5.54	123.22	119.90
1	A	926	G	N1-C2-N2	-5.54	111.21	116.20
1	A	1302	U	C6-N1-C1'	-5.54	113.45	121.20
1	A	543	C	C5-C4-N4	5.53	124.07	120.20
1	A	1373	G	N3-C4-N9	5.53	129.32	126.00
1	A	578	C	N3-C2-O2	-5.53	118.03	121.90
1	A	486	U	C5-C6-N1	5.52	125.46	122.70
4	D	202	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	839	U	N3-C2-O2	-5.52	118.34	122.20
1	A	649	G	C6-C5-N7	-5.51	127.09	130.40
1	A	906	G	C6-C5-N7	-5.51	127.09	130.40
1	A	381	C	C6-N1-C2	-5.51	118.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1072	G	C4-N9-C1'	5.51	133.66	126.50
1	A	113	G	N3-C4-C5	-5.50	125.85	128.60
1	A	546	G	C4-N9-C1'	5.50	133.65	126.50
1	A	427	U	N1-C2-O2	5.50	126.65	122.80
1	A	22	G	N3-C4-C5	5.50	131.35	128.60
1	A	916	G	N7-C8-N9	5.49	115.85	113.10
1	A	849	C	C6-N1-C2	-5.49	118.10	120.30
1	A	1507	A	N1-C2-N3	5.49	132.05	129.30
1	A	1526	G	N3-C4-C5	-5.49	125.86	128.60
1	A	878	G	C8-N9-C1'	-5.49	119.87	127.00
8	H	43	GLY	N-CA-C	5.49	126.81	113.10
1	A	822	C	N3-C2-O2	-5.48	118.06	121.90
1	A	1106	G	C8-N9-C4	-5.48	104.21	106.40
1	A	943	U	C5-C6-N1	5.48	125.44	122.70
1	A	362	G	C5-N7-C8	-5.48	101.56	104.30
1	A	1079	G	C5-C6-O6	-5.47	125.32	128.60
1	A	1527	C	N1-C2-O2	-5.46	115.62	118.90
1	A	125	U	N3-C4-O4	5.46	123.22	119.40
1	A	660	G	N7-C8-N9	5.46	115.83	113.10
1	A	566	G	C5-C6-O6	5.46	131.87	128.60
1	A	651	C	N3-C4-C5	-5.45	119.72	121.90
1	A	891	U	C5-C6-N1	5.44	125.42	122.70
1	A	872	A	N7-C8-N9	5.43	116.52	113.80
4	D	14	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	110	C	N1-C2-O2	5.43	122.16	118.90
1	A	335	C	C6-N1-C2	-5.43	118.13	120.30
1	A	659	U	C5-C6-N1	5.43	125.41	122.70
1	A	765	G	C8-N9-C4	-5.43	104.23	106.40
1	A	878	G	C4-N9-C1'	5.42	133.55	126.50
1	A	840	C	N3-C2-O2	-5.42	118.11	121.90
1	A	496	A	N1-C6-N6	-5.42	115.35	118.60
1	A	501	C	N3-C2-O2	-5.42	118.11	121.90
1	A	655	A	C6-N1-C2	-5.42	115.35	118.60
1	A	18	C	C5-C6-N1	5.41	123.70	121.00
1	A	1203	C	C5-C6-N1	5.41	123.70	121.00
1	A	563	A	C4-C5-N7	5.41	113.40	110.70
1	A	816	A	C5-C6-N1	-5.41	115.00	117.70
1	A	1239	A	C8-N9-C4	5.40	107.96	105.80
1	A	763	G	C8-N9-C4	-5.40	104.24	106.40
1	A	971	G	C5-C6-O6	5.40	131.84	128.60
1	A	730	G	N7-C8-N9	5.39	115.80	113.10
1	A	110	C	N3-C4-C5	-5.39	119.74	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	489	C	C5-C6-N1	5.39	123.70	121.00
1	A	1158	C	N3-C2-O2	-5.39	118.13	121.90
1	A	8	A	N9-C4-C5	5.38	107.95	105.80
1	A	878	G	C6-C5-N7	-5.38	127.17	130.40
1	A	1093	A	C8-N9-C4	-5.38	103.65	105.80
1	A	96	G	C8-N9-C4	-5.38	104.25	106.40
1	A	609	A	N1-C6-N6	5.38	121.83	118.60
1	A	863	U	N1-C2-N3	5.38	118.13	114.90
1	A	1128	C	C6-N1-C2	-5.38	118.15	120.30
1	A	635	G	N3-C4-C5	5.37	131.29	128.60
1	A	811	C	N1-C2-O2	5.37	122.12	118.90
1	A	1366	C	C6-N1-C2	-5.37	118.15	120.30
1	A	564	C	N3-C4-C5	-5.37	119.75	121.90
1	A	312	C	N1-C2-O2	5.37	122.12	118.90
1	A	721	G	N3-C4-N9	5.36	129.22	126.00
1	A	880	C	C6-N1-C2	5.36	122.44	120.30
1	A	552	U	N3-C4-O4	-5.36	115.65	119.40
1	A	1185	G	N7-C8-N9	5.36	115.78	113.10
1	A	799	G	C8-N9-C4	-5.35	104.26	106.40
1	A	916	G	C4-N9-C1'	5.35	133.46	126.50
1	A	91	C	C6-N1-C2	5.35	122.44	120.30
1	A	19	C	N1-C2-O2	5.35	122.11	118.90
1	A	203	U	C6-N1-C2	-5.35	117.79	121.00
1	A	1403	C	C5-C6-N1	5.35	123.67	121.00
1	A	1354	C	C5-C6-N1	5.34	123.67	121.00
1	A	426	G	N3-C4-C5	-5.34	125.93	128.60
1	A	825	G	N3-C4-C5	-5.34	125.93	128.60
1	A	661	G	C8-N9-C4	-5.34	104.27	106.40
1	A	1525	G	C8-N9-C4	-5.33	104.27	106.40
1	A	930	C	N3-C4-C5	-5.32	119.77	121.90
1	A	870	U	C2-N1-C1'	-5.32	111.31	117.70
1	A	801	U	C6-N1-C2	-5.32	117.81	121.00
1	A	501	C	N1-C2-O2	5.31	122.09	118.90
1	A	285	G	C2-N3-C4	-5.31	109.25	111.90
1	A	979	C	C6-N1-C2	-5.29	118.18	120.30
1	A	817	C	C6-N1-C2	-5.29	118.18	120.30
1	A	407	G	C8-N9-C1'	5.29	133.87	127.00
1	A	866	C	N1-C2-O2	5.28	122.07	118.90
1	A	801	U	C5-C6-N1	5.28	125.34	122.70
1	A	1045	C	C5-C6-N1	5.28	123.64	121.00
1	A	816	A	C8-N9-C4	-5.27	103.69	105.80
1	A	281	G	N3-C4-C5	-5.26	125.97	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	563	A	C6-C5-N7	-5.26	128.62	132.30
1	A	740	U	C6-N1-C1'	5.26	128.56	121.20
1	A	755	G	N1-C6-O6	5.26	123.06	119.90
1	A	121	C	C6-N1-C2	-5.26	118.20	120.30
1	A	1096	C	N3-C4-N4	5.25	121.68	118.00
1	A	863	U	N3-C4-C5	-5.24	111.45	114.60
1	A	883	C	C6-N1-C2	-5.24	118.20	120.30
1	A	994	A	N7-C8-N9	5.24	116.42	113.80
1	A	1520	G	C8-N9-C4	-5.24	104.30	106.40
1	A	271	C	C6-N1-C2	-5.24	118.21	120.30
1	A	1039	C	C6-N1-C2	5.23	122.39	120.30
1	A	1441	G	C8-N9-C4	-5.22	104.31	106.40
1	A	599	C	C6-N1-C2	5.21	122.38	120.30
1	A	732	C	N1-C2-O2	5.21	122.03	118.90
8	H	10	LEU	CA-CB-CG	-5.21	103.32	115.30
1	A	1107	C	N3-C4-N4	5.21	121.64	118.00
1	A	1290	G	C8-N9-C4	-5.21	104.32	106.40
14	N	6	LEU	CA-CB-CG	-5.21	103.33	115.30
1	A	1354	C	C6-N1-C2	-5.20	118.22	120.30
1	A	811	C	C6-N1-C2	-5.20	118.22	120.30
1	A	433	C	C2-N1-C1'	5.20	124.52	118.80
1	A	838	G	C8-N9-C4	-5.20	104.32	106.40
1	A	615	C	C2-N3-C4	5.19	122.50	119.90
1	A	826	C	C6-N1-C2	-5.19	118.22	120.30
1	A	572	A	C4-C5-N7	-5.19	108.11	110.70
1	A	384	G	C8-N9-C4	-5.18	104.33	106.40
1	A	73	C	C5-C6-N1	5.17	123.59	121.00
6	F	43	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	816	A	C4-C5-N7	-5.17	108.11	110.70
1	A	854	G	C5-C6-O6	-5.17	125.50	128.60
1	A	725	G	C4-C5-N7	5.16	112.86	110.80
1	A	1081	G	C8-N9-C1'	5.16	133.71	127.00
1	A	1168	A	N9-C4-C5	5.16	107.87	105.80
1	A	801	U	C2-N1-C1'	5.16	123.89	117.70
1	A	819	A	C5-C6-N6	-5.16	119.58	123.70
1	A	882	C	N3-C4-C5	5.16	123.96	121.90
1	A	388	G	C4-N9-C1'	-5.15	119.80	126.50
1	A	197	A	N1-C6-N6	-5.15	115.51	118.60
1	A	836	G	C6-C5-N7	-5.15	127.31	130.40
1	A	979	C	N3-C4-C5	-5.15	119.84	121.90
1	A	581	G	N3-C2-N2	-5.14	116.30	119.90
1	A	1077	G	N7-C8-N9	5.14	115.67	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1402	C	C5-C6-N1	5.14	123.57	121.00
1	A	849	C	C5-C6-N1	5.14	123.57	121.00
1	A	800	G	N7-C8-N9	5.14	115.67	113.10
1	A	894	G	N3-C4-C5	5.14	131.17	128.60
1	A	938	A	N7-C8-N9	5.14	116.37	113.80
1	A	929	G	N3-C2-N2	-5.13	116.31	119.90
1	A	1083	U	C5-C6-N1	5.13	125.27	122.70
1	A	1088	G	C8-N9-C4	-5.13	104.35	106.40
1	A	1108	G	C2-N3-C4	5.12	114.46	111.90
1	A	1515	C	C5-C6-N1	5.12	123.56	121.00
1	A	618	C	C2-N1-C1'	5.12	124.43	118.80
1	A	1259	C	C6-N1-C2	-5.12	118.25	120.30
1	A	545	C	C2-N1-C1'	5.12	124.43	118.80
1	A	1093	A	C6-C5-N7	-5.12	128.72	132.30
1	A	882	C	C5-C6-N1	-5.11	118.44	121.00
1	A	1237	C	C6-N1-C2	-5.11	118.25	120.30
1	A	27	G	C5-C6-O6	-5.11	125.53	128.60
1	A	769	G	N3-C4-C5	5.11	131.16	128.60
1	A	775	G	C8-N9-C4	-5.11	104.36	106.40
1	A	305	G	N3-C4-C5	-5.11	126.05	128.60
1	A	728	A	C5-C6-N1	5.10	120.25	117.70
1	A	335	C	C5-C6-N1	5.10	123.55	121.00
1	A	744	C	N3-C4-N4	5.10	121.57	118.00
1	A	547	A	N3-C4-C5	-5.10	123.23	126.80
1	A	1435	G	C5-C6-N1	-5.10	108.95	111.50
1	A	672	U	C5-C4-O4	-5.10	122.84	125.90
1	A	920	U	N3-C4-C5	-5.09	111.55	114.60
1	A	654	G	C8-N9-C4	5.09	108.44	106.40
1	A	516	U	N1-C2-N3	5.08	117.95	114.90
1	A	657	G	N1-C6-O6	5.08	122.95	119.90
1	A	1168	A	N1-C6-N6	-5.08	115.55	118.60
1	A	410	G	C8-N9-C1'	-5.08	120.40	127.00
1	A	874	G	C6-C5-N7	-5.08	127.35	130.40
1	A	1077	G	C4-N9-C1'	5.08	133.10	126.50
1	A	1232	U	N1-C2-N3	5.08	117.95	114.90
1	A	749	C	N3-C2-O2	-5.08	118.35	121.90
1	A	864	A	C5-C6-N1	5.08	120.24	117.70
1	A	1515	C	C6-N1-C2	-5.08	118.27	120.30
1	A	886	G	N1-C6-O6	5.07	122.94	119.90
1	A	1367	C	N3-C4-C5	-5.07	119.87	121.90
1	A	137	C	C6-N1-C2	-5.07	118.27	120.30
1	A	666	G	C4-C5-N7	5.07	112.83	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1223	C	N1-C2-O2	5.07	121.94	118.90
1	A	1532	U	C6-N1-C2	-5.07	117.96	121.00
1	A	784	C	N3-C4-C5	5.07	123.93	121.90
1	A	917	G	N9-C4-C5	5.07	107.43	105.40
4	D	88	VAL	CB-CA-C	-5.07	101.78	111.40
1	A	1066	C	N3-C2-O2	5.06	125.44	121.90
1	A	1389	C	C6-N1-C2	-5.06	118.28	120.30
1	A	711	G	C8-N9-C4	-5.06	104.38	106.40
1	A	673	G	N1-C6-O6	5.05	122.93	119.90
1	A	863	U	C6-N1-C2	-5.05	117.97	121.00
1	A	797	C	C5-C6-N1	5.04	123.52	121.00
1	A	902	G	C8-N9-C4	5.04	108.42	106.40
1	A	735	C	C6-N1-C2	-5.04	118.28	120.30
1	A	1392	G	C2-N3-C4	5.04	114.42	111.90
4	D	94	LEU	CA-CB-CG	-5.04	103.71	115.30
8	H	104	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	551	U	C6-N1-C2	5.04	124.02	121.00
1	A	407	G	N7-C8-N9	5.03	115.62	113.10
1	A	531	U	C6-N1-C2	-5.03	117.98	121.00
1	A	1093	A	C4-N9-C1'	5.03	135.36	126.30
1	A	891	U	N3-C4-C5	-5.03	111.58	114.60
1	A	124	G	C4-N9-C1'	5.03	133.04	126.50
1	A	1047	G	N1-C6-O6	5.02	122.92	119.90
1	A	1365	G	C8-N9-C4	-5.02	104.39	106.40
1	A	801	U	N3-C4-O4	5.02	122.92	119.40
1	A	596	C	C6-N1-C2	5.01	122.31	120.30
1	A	1068	G	C8-N9-C4	-5.01	104.39	106.40
1	A	369	C	C6-N1-C2	-5.01	118.30	120.30
1	A	896	C	N3-C4-C5	5.01	123.91	121.90
1	A	576	G	C4-C5-N7	5.01	112.80	110.80
1	A	980	C	C5-C4-N4	5.01	123.70	120.20
1	A	1344	C	C5-C6-N1	5.00	123.50	121.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	28	SER	Peptide
4	D	31	CYS	Peptide
6	F	2	ARG	Peptide
6	F	46	ARG	Peptide
12	L	126	LYS	Peptide

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Mol	Chain	Res	Type	Group
17	Q	100	LYS	Peptide
17	Q	32	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32392	0	16349	1113	0
2	B	1842	0	1894	118	0
3	C	1613	0	1677	107	0
4	D	1703	0	1763	135	0
5	E	1199	0	1251	100	0
6	F	843	0	857	78	0
7	G	1257	0	1296	52	0
8	H	1116	0	1177	94	0
9	I	1010	0	1037	52	0
10	J	802	0	849	47	0
11	K	854	0	868	42	0
12	L	971	0	1057	67	0
13	M	947	0	1008	36	0
14	N	492	0	532	34	0
15	O	734	0	771	46	0
16	P	717	0	738	38	0
17	Q	857	0	928	47	0
18	R	598	0	670	46	0
19	S	666	0	686	28	0
20	T	763	0	861	39	0
21	V	209	0	221	7	0
22	A	42	0	38	1	0
23	A	102	0	0	0	0
23	E	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
All	All	51732	0	36528	2073	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (2073) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:A:OP1	5:E:126:ARG:NH2	1.92	1.01
17:Q:29:HIS:HB3	17:Q:33:GLY:H	1.27	0.98
1:A:447:G:H2'	1:A:485:G:H22	1.28	0.97
1:A:663:A:H2'	1:A:664:G:H8	1.29	0.96
2:B:100:GLY:O	2:B:102:LEU:N	2.00	0.95
8:H:109:ILE:HD11	8:H:120:THR:HB	1.49	0.93
18:R:58:LEU:HD13	18:R:62:GLU:HB3	1.52	0.92
1:A:947:G:N2	1:A:1235:U:O2	2.03	0.92
6:F:50:TYR:CE2	18:R:77:GLY:HA2	2.06	0.89
1:A:869:G:H4'	1:A:872:A:C8	2.08	0.88
1:A:316:G:H1	1:A:337:C:H42	1.21	0.88
6:F:4:TYR:HD2	6:F:4:TYR:H	1.12	0.88
4:D:119:GLN:HE21	4:D:123:HIS:HE1	1.17	0.88
1:A:1347:G:HO2'	1:A:1373:G:H1	1.19	0.87
1:A:1256:A:OP2	3:C:26:LYS:NZ	2.06	0.87
3:C:127:ARG:HH21	3:C:191:THR:HG22	1.36	0.87
4:D:59:ARG:HE	4:D:59:ARG:HA	1.40	0.86
1:A:42:G:N2	1:A:401:C:O2	2.09	0.85
6:F:50:TYR:HE2	18:R:77:GLY:HA2	1.40	0.84
11:K:43:SER:HB3	11:K:68:ALA:HB2	1.59	0.84
1:A:1305:G:H22	1:A:1331:G:H1'	1.40	0.84
1:A:779:C:H42	1:A:803:G:H1	1.22	0.84
1:A:677:U:H3	1:A:714:G:H22	1.26	0.83
1:A:1055:A:H62	1:A:1200:C:H42	1.26	0.83
15:O:33:THR:O	15:O:37:ASN:ND2	2.11	0.83
1:A:978:A:O2'	1:A:1322:C:N3	2.11	0.83
1:A:582:U:H2'	1:A:583:A:H8	1.42	0.82
3:C:40:ARG:NH1	3:C:55:VAL:O	2.11	0.82
5:E:152:ARG:O	5:E:154:GLY:N	2.12	0.82
1:A:663:A:H2'	1:A:664:G:C8	2.15	0.82
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.62	0.82
1:A:108:G:H5'	1:A:110:C:H5	1.45	0.82
2:B:4:GLU:O	2:B:217:ARG:NH1	2.13	0.81
1:A:1417:G:O2'	1:A:1483:A:N6	2.12	0.81
6:F:82:ARG:H	6:F:82:ARG:HD2	1.43	0.81
1:A:8:A:H1'	5:E:103:GLY:HA2	1.61	0.81
1:A:501:C:O2	1:A:549:C:O2'	1.98	0.81
5:E:36:ASP:O	5:E:38:GLN:N	2.13	0.81
17:Q:64:PRO:HB3	17:Q:70:ARG:HH11	1.46	0.81
4:D:5:ILE:HA	4:D:115:ARG:HH22	1.46	0.81
1:A:409:G:H2'	1:A:410:G:H8	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:10:GLY:HA3	10:J:16:LEU:HD21	1.64	0.79
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.65	0.79
1:A:594:G:O6	1:A:645:C:N4	2.14	0.79
16:P:6:LEU:HB3	16:P:17:TYR:HD2	1.48	0.79
4:D:9:CYS:SG	4:D:32:ALA:N	2.54	0.79
1:A:1305:G:N2	1:A:1331:G:H1'	1.98	0.78
1:A:979:C:H2'	1:A:980:C:H5'	1.65	0.78
1:A:398:C:H2'	1:A:399:G:H8	1.47	0.78
1:A:1505:G:H4'	1:A:1506:U:H5"	1.66	0.77
1:A:651:C:H2'	1:A:652:U:C6	2.19	0.77
1:A:770:C:O2	1:A:899:C:N4	2.16	0.77
1:A:581:G:OP1	15:O:65:ARG:NH2	2.18	0.77
1:A:545:C:OP1	4:D:61:LYS:NZ	2.18	0.77
18:R:48:GLY:O	18:R:74:ARG:NH2	2.18	0.77
8:H:17:THR:O	8:H:19:VAL:N	2.18	0.77
1:A:765:G:N2	1:A:812:C:H1'	1.99	0.77
12:L:60:LEU:HD12	12:L:64:TYR:HB2	1.66	0.77
6:F:68:PRO:HB2	6:F:71:ARG:HD2	1.67	0.77
1:A:375:U:H4'	16:P:17:TYR:HE2	1.50	0.77
8:H:114:THR:OG1	8:H:117:GLY:N	2.17	0.77
1:A:382:A:H2'	1:A:383:A:H8	1.50	0.77
1:A:1065:U:H5	1:A:1190:G:C8	2.03	0.76
2:B:103:THR:OG1	2:B:103:THR:O	2.03	0.76
1:A:426:G:OP1	4:D:38:TYR:OH	2.04	0.76
1:A:765:G:H21	1:A:813:U:H5	1.31	0.76
2:B:102:LEU:HB3	2:B:180:LEU:HD11	1.67	0.76
1:A:1071:C:H2'	1:A:1072:G:H8	1.50	0.76
1:A:1060:C:H5	3:C:2:GLY:HA3	1.51	0.76
1:A:17:U:H2'	1:A:18:C:H6	1.51	0.76
1:A:591:U:H2'	1:A:592:G:H8	1.51	0.75
1:A:509:A:N7	1:A:510:A:C6	2.55	0.75
1:A:938:A:N3	1:A:1376:U:O2'	2.19	0.75
1:A:575:G:O4'	1:A:881:G:N2	2.20	0.75
3:C:35:GLU:OE2	3:C:59:ARG:NH2	2.19	0.75
1:A:1366:C:H2'	1:A:1367:C:H6	1.52	0.75
12:L:5:PRO:HG2	12:L:10:LEU:HD21	1.67	0.75
3:C:130:VAL:HG11	3:C:157:ILE:HG23	1.68	0.75
20:T:90:GLN:HA	20:T:93:GLU:HG2	1.68	0.74
1:A:878:G:H2'	1:A:879:C:H6	1.52	0.74
1:A:831:U:H5'	2:B:22:LYS:HG3	1.67	0.74
1:A:1152:A:H5'	10:J:13:HIS:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:A:H2'	1:A:11:G:H8	1.53	0.74
1:A:1326:C:OP1	21:V:12:LYS:NZ	2.19	0.74
8:H:93:VAL:HG12	8:H:133:LEU:HB3	1.70	0.74
17:Q:7:THR:HG23	17:Q:58:GLU:HG3	1.69	0.74
6:F:4:TYR:CD2	6:F:4:TYR:N	2.53	0.74
1:A:501:C:OP1	12:L:117:ARG:NH2	2.21	0.74
1:A:577:G:C2	1:A:578:C:C5	2.75	0.74
8:H:14:ARG:O	8:H:17:THR:OG1	2.06	0.74
18:R:76:LEU:O	18:R:78:LEU:N	2.18	0.74
1:A:481:G:O2'	1:A:483:C:N4	2.19	0.74
3:C:7:PRO:HG2	3:C:184:TYR:HB2	1.70	0.74
1:A:651:C:H2'	1:A:652:U:H6	1.53	0.73
1:A:1077:G:N2	1:A:1079:G:H3'	2.02	0.73
9:I:110:GLU:OE2	9:I:113:LYS:NZ	2.22	0.73
1:A:1347:G:C8	9:I:107:ARG:HB3	2.23	0.73
1:A:1187:G:H2'	1:A:1188:A:H8	1.53	0.73
1:A:1072:G:OP1	5:E:57:LYS:NZ	2.22	0.72
1:A:582:U:H2'	1:A:583:A:C8	2.23	0.72
4:D:94:LEU:O	4:D:97:LEU:N	2.22	0.72
1:A:533:A:O2'	1:A:535:A:OP2	2.07	0.72
2:B:178:ARG:HG3	8:H:72:PRO:HA	1.71	0.72
1:A:1124:G:H5"	10:J:35:SER:HB2	1.70	0.72
2:B:181:PHE:HD1	2:B:181:PHE:H	1.36	0.72
1:A:674:G:H2'	1:A:675:A:H8	1.54	0.72
1:A:427:U:H5"	1:A:428:G:H2'	1.72	0.72
1:A:669:U:H3	1:A:737:A:H61	1.37	0.72
1:A:95:U:H2'	1:A:96:G:C8	2.24	0.72
1:A:720:C:H4'	18:R:63:GLN:HE21	1.55	0.72
7:G:27:ILE:HD13	7:G:40:ALA:HA	1.72	0.72
6:F:18:GLN:HA	6:F:21:LEU:HB3	1.72	0.72
1:A:66:G:N7	1:A:104:G:N2	2.38	0.72
8:H:17:THR:O	8:H:20:TYR:N	2.13	0.71
1:A:1103:C:H5'	2:B:98:LEU:HD22	1.72	0.71
1:A:620:C:O2	4:D:137:SER:OG	2.07	0.71
2:B:115:LEU:HD21	2:B:153:ARG:HH21	1.55	0.71
8:H:114:THR:HG21	8:H:119:LEU:HD12	1.71	0.71
1:A:571:U:H3'	1:A:572:A:H5"	1.72	0.71
9:I:116:LYS:O	9:I:118:LYS:N	2.24	0.71
1:A:1422:G:H2'	1:A:1423:G:H8	1.55	0.71
6:F:66:GLU:HG3	6:F:67:MET:H	1.53	0.71
1:A:675:A:H2'	1:A:676:A:H8	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:101:LEU:HB2	4:D:138:TYR:HB3	1.72	0.71
1:A:869:G:O2'	1:A:872:A:N7	2.17	0.71
12:L:74:GLY:O	12:L:102:ARG:NH1	2.18	0.71
1:A:737:A:H2'	1:A:738:C:C6	2.26	0.71
1:A:108:G:H5'	1:A:110:C:C5	2.26	0.71
4:D:64:LEU:HB2	4:D:198:VAL:HG11	1.71	0.70
1:A:296:U:H2'	1:A:297:G:H8	1.55	0.70
2:B:29:ALA:O	2:B:31:TYR:N	2.24	0.70
3:C:175:LEU:HD23	3:C:175:LEU:H	1.55	0.70
1:A:891:U:H2'	1:A:892:A:H8	1.55	0.70
1:A:7:G:H2'	5:E:119:LEU:HD23	1.73	0.70
1:A:113:G:H1'	1:A:354:G:H5'	1.74	0.70
4:D:108:LEU:HD11	4:D:183:GLY:HA3	1.73	0.70
1:A:304:U:H2'	1:A:305:G:C8	2.25	0.70
1:A:920:U:H2'	1:A:921:U:C6	2.27	0.70
5:E:144:THR:O	5:E:146:ALA:N	2.25	0.70
7:G:139:GLU:O	7:G:143:ARG:NH1	2.25	0.70
1:A:1022:G:H2'	1:A:1023:G:H8	1.57	0.70
1:A:667:G:O2'	15:O:49:ASP:OD1	2.06	0.70
4:D:163:GLU:O	4:D:165:MET:N	2.24	0.70
5:E:126:ARG:HA	5:E:131:ILE:HD11	1.74	0.70
2:B:122:PHE:HA	2:B:127:ILE:HD13	1.73	0.69
9:I:18:PHE:HB2	9:I:62:TYR:HB3	1.72	0.69
21:V:8:THR:OG1	21:V:9:ARG:N	2.22	0.69
12:L:89:ARG:HG2	12:L:90:VAL:H	1.57	0.69
12:L:49:ASN:ND2	12:L:92:ASP:OD1	2.25	0.69
4:D:24:GLU:HB2	4:D:112:VAL:HG13	1.74	0.69
13:M:14:ARG:HB3	13:M:17:VAL:HG23	1.73	0.69
9:I:35:GLU:HA	9:I:38:GLN:HE21	1.57	0.69
1:A:8:A:N7	4:D:208:SER:OG	2.24	0.69
1:A:601:C:H2'	1:A:602:A:H8	1.58	0.69
1:A:447:G:H2'	1:A:485:G:N2	2.06	0.69
1:A:1182:G:H4'	1:A:1183:A:H5"	1.74	0.69
13:M:79:LYS:NZ	13:M:83:ASP:OD2	2.15	0.69
5:E:52:PRO:HA	5:E:55:VAL:HG23	1.75	0.69
1:A:375:U:H4'	16:P:17:TYR:CE2	2.28	0.69
10:J:42:THR:HG22	10:J:68:HIS:HA	1.74	0.69
4:D:79:PHE:HZ	4:D:204:ILE:HG23	1.55	0.69
1:A:739:C:H3'	1:A:739:C:H6	1.58	0.68
2:B:42:ILE:HG22	2:B:44:LEU:HD23	1.73	0.68
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.75	0.68
3:C:127:ARG:NH2	3:C:191:THR:HG22	2.08	0.68
1:A:675:A:H2'	1:A:676:A:C8	2.29	0.68
4:D:171:GLY:O	4:D:173:TRP:N	2.27	0.68
4:D:18:LYS:HZ3	4:D:31:CYS:HB3	1.58	0.68
2:B:61:LEU:O	2:B:66:GLY:N	2.27	0.68
6:F:23:LYS:O	6:F:27:GLN:HG2	1.94	0.68
2:B:54:THR:HG23	2:B:199:TYR:HB3	1.75	0.68
19:S:30:LEU:HD13	19:S:48:THR:HG22	1.76	0.68
17:Q:93:GLN:O	17:Q:95:TYR:N	2.27	0.68
1:A:128:G:H4'	17:Q:3:LYS:HG2	1.74	0.68
5:E:99:GLY:HA2	5:E:117:ASP:HA	1.76	0.68
4:D:59:ARG:NE	4:D:59:ARG:HA	2.08	0.68
4:D:105:VAL:O	4:D:108:LEU:N	2.25	0.68
1:A:149:A:H2'	1:A:150:C:H6	1.59	0.68
1:A:3:G:N2	1:A:5:U:O2'	2.27	0.68
1:A:818:G:O2'	1:A:819:A:H5'	1.94	0.67
2:B:152:PHE:HE1	2:B:155:LEU:HD12	1.59	0.67
1:A:410:G:OP1	4:D:30:LYS:NZ	2.27	0.67
16:P:53:VAL:HG13	16:P:79:VAL:HA	1.77	0.67
1:A:828:A:N3	2:B:26:PRO:HG2	2.09	0.67
1:A:235:C:H2'	1:A:236:G:H8	1.58	0.67
6:F:66:GLU:HG3	6:F:67:MET:N	2.09	0.67
1:A:892:A:O2'	1:A:1415:G:H4'	1.94	0.67
1:A:242:C:N3	1:A:285:G:N2	2.43	0.67
1:A:743:U:H2'	1:A:744:C:C6	2.29	0.67
1:A:779:C:N4	1:A:803:G:H1	1.91	0.67
10:J:90:LEU:H	10:J:91:PRO:HD2	1.59	0.67
8:H:44:PHE:HB3	8:H:80:ILE:HD13	1.77	0.67
4:D:119:GLN:HE21	4:D:123:HIS:CE1	2.08	0.67
1:A:1422:G:H2'	1:A:1423:G:C8	2.30	0.67
3:C:136:GLN:HA	3:C:139:GLN:HB2	1.77	0.67
1:A:183:G:N2	1:A:223:U:O2'	2.21	0.67
1:A:1348:U:H4'	9:I:120:ARG:HG3	1.77	0.67
1:A:689:C:OP1	11:K:44:SER:OG	2.12	0.67
1:A:1415:G:N2	1:A:1485:U:O2	2.26	0.66
15:O:69:TYR:HE1	15:O:73:GLU:HG3	1.60	0.66
1:A:922:G:H2'	1:A:923:A:C8	2.30	0.66
6:F:48:LEU:HD13	6:F:52:ILE:HG13	1.77	0.66
1:A:910:C:H2'	1:A:911:U:H6	1.61	0.66
1:A:1003:G:N2	1:A:1038:C:O2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:A:N6	1:A:1200:C:H42	1.91	0.66
9:I:28:VAL:HA	9:I:63:ILE:HB	1.78	0.66
1:A:865:A:N3	1:A:918:A:O2'	2.25	0.66
7:G:115:ARG:HB3	7:G:118:VAL:HB	1.77	0.66
1:A:875:C:H1'	8:H:15:ASN:HD21	1.59	0.66
4:D:25:ARG:O	4:D:28:SER:OG	2.06	0.66
1:A:821:G:C2'	1:A:822:C:H5'	2.26	0.66
3:C:121:ALA:HA	3:C:124:ILE:HD12	1.77	0.66
17:Q:90:ILE:O	17:Q:94:ASN:ND2	2.26	0.66
1:A:958:A:N6	19:S:77:THR:O	2.28	0.66
2:B:82:ARG:NE	2:B:92:TYR:OH	2.27	0.66
1:A:746:A:H2'	1:A:747:C:H6	1.59	0.66
1:A:523:A:H61	12:L:92:ASP:HB2	1.60	0.66
1:A:1223:C:OP1	19:S:78:ARG:NH1	2.28	0.66
16:P:32:TYR:HE2	16:P:35:LYS:HB2	1.61	0.66
1:A:880:C:OP1	12:L:12:ARG:NH2	2.27	0.66
1:A:1187:G:H2'	1:A:1188:A:C8	2.31	0.66
1:A:1353:G:N2	1:A:1369:C:O2	2.29	0.65
20:T:50:GLU:HB2	20:T:99:LEU:HD12	1.77	0.65
1:A:1311:G:N2	1:A:1326:C:O2	2.29	0.65
4:D:11:LEU:HA	4:D:14:ARG:H	1.62	0.65
1:A:771:G:N3	1:A:809:G:N2	2.44	0.65
4:D:9:CYS:HA	4:D:12:CYS:HB2	1.79	0.65
13:M:108:ARG:HH22	13:M:111:LYS:HD2	1.61	0.65
13:M:102:ARG:NH1	13:M:105:THR:OG1	2.26	0.65
1:A:1350:A:OP1	9:I:121:ARG:NH1	2.30	0.65
15:O:26:GLU:HG3	15:O:81:LEU:HD22	1.78	0.65
7:G:111:ARG:HD2	7:G:123:GLU:HB2	1.79	0.65
1:A:872:A:N3	1:A:874:G:C5	2.65	0.65
8:H:106:GLY:O	8:H:122:ARG:NH2	2.30	0.65
2:B:61:LEU:HD21	2:B:160:ASP:HB2	1.79	0.65
1:A:1416:G:N2	1:A:1484:C:O2	2.29	0.65
1:A:171:A:H2'	1:A:172:A:C8	2.32	0.65
11:K:21:ILE:HB	11:K:84:VAL:HG12	1.79	0.65
13:M:91:ARG:HB2	13:M:98:VAL:HG22	1.78	0.65
1:A:1377:A:OP2	7:G:94:ARG:NH2	2.21	0.64
4:D:26:CYS:HA	4:D:31:CYS:CB	2.27	0.64
2:B:88:ALA:HA	2:B:223:ILE:HD11	1.80	0.64
8:H:34:GLU:HB3	8:H:118:VAL:HG21	1.80	0.64
6:F:67:MET:SD	6:F:75:LEU:HD23	2.37	0.64
1:A:1065:U:C5	1:A:1190:G:C8	2.86	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:G:H1	1:A:1149:C:H42	1.46	0.64
1:A:63:C:H42	1:A:104:G:H1	1.42	0.64
1:A:1228:C:H2'	1:A:1229:A:C8	2.33	0.64
11:K:19:ALA:HB3	11:K:82:VAL:HG13	1.79	0.64
1:A:1145:C:H4'	1:A:1146:A:O5'	1.98	0.64
1:A:568:G:N2	1:A:883:C:O2	2.30	0.64
19:S:19:VAL:HG11	19:S:44:MET:HG2	1.78	0.64
1:A:1314:C:H2'	1:A:1315:U:H6	1.63	0.64
1:A:410:G:N2	1:A:429:U:O2	2.31	0.64
1:A:803:G:H2'	1:A:804:U:C6	2.33	0.64
3:C:39:ILE:O	3:C:43:LEU:HB2	1.97	0.64
1:A:1194:U:H2'	1:A:1195:C:C6	2.32	0.64
1:A:1068:G:N2	1:A:1191:A:N3	2.42	0.64
1:A:736:C:H2'	1:A:737:A:C8	2.33	0.64
1:A:1414:U:H2'	1:A:1415:G:C8	2.33	0.64
1:A:504:C:H1'	1:A:510:A:C4	2.33	0.64
1:A:627:G:OP2	16:P:35:LYS:NZ	2.31	0.64
19:S:44:MET:HA	19:S:47:HIS:HD2	1.63	0.64
1:A:703:G:H4'	1:A:704:A:H5'	1.80	0.64
9:I:13:ALA:HB2	9:I:68:GLY:HA3	1.80	0.64
11:K:92:GLU:HG2	11:K:95:ILE:HD12	1.80	0.64
12:L:7:ILE:O	12:L:11:VAL:HG23	1.98	0.64
20:T:46:GLU:HB2	20:T:48:LYS:HE3	1.80	0.64
1:A:403:C:O2'	4:D:122:ARG:NH2	2.31	0.64
1:A:821:G:H2'	1:A:822:C:H5'	1.80	0.63
1:A:171:A:H2'	1:A:172:A:H8	1.63	0.63
1:A:932:C:H2'	1:A:933:G:C8	2.33	0.63
9:I:53:VAL:HG12	9:I:95:LYS:HD2	1.79	0.63
1:A:8:A:C5	4:D:209:ARG:HB2	2.33	0.63
2:B:155:LEU:HD11	2:B:159:PRO:HD3	1.80	0.63
1:A:324:G:N2	1:A:327:A:C8	2.67	0.63
1:A:1347:G:H8	9:I:107:ARG:HB3	1.64	0.63
1:A:730:G:N3	1:A:765:G:H4'	2.14	0.63
6:F:5:GLU:HB3	6:F:62:TRP:HE1	1.63	0.63
1:A:1105:A:H2'	1:A:1106:G:H8	1.63	0.63
8:H:36:LEU:HD12	8:H:48:TYR:HB3	1.80	0.63
1:A:571:U:H3'	1:A:572:A:C5'	2.28	0.63
14:N:45:ARG:O	14:N:48:ALA:N	2.31	0.63
4:D:103:ASN:O	4:D:103:ASN:ND2	2.29	0.63
11:K:112:THR:O	11:K:114:VAL:HG23	1.99	0.63
4:D:41:GLY:O	4:D:43:HIS:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1298:C:C5	7:G:114:ARG:HD3	2.33	0.63
2:B:47:THR:O	2:B:51:LEU:HB2	1.98	0.63
2:B:149:LEU:O	2:B:152:PHE:N	2.31	0.63
1:A:1091:U:H2'	1:A:1093:A:OP2	1.98	0.63
4:D:109:GLY:O	4:D:111:ALA:N	2.22	0.63
1:A:724:G:C2	1:A:725:G:C8	2.86	0.63
12:L:105:TYR:O	12:L:107:ALA:N	2.27	0.62
15:O:35:ARG:NH2	15:O:59:MET:SD	2.71	0.62
4:D:96:LEU:HB3	4:D:139:ARG:HH12	1.64	0.62
1:A:1095:U:H2'	1:A:1096:C:O4'	1.99	0.62
1:A:746:A:H2'	1:A:747:C:C6	2.34	0.62
1:A:994:A:N7	1:A:1216:G:H4'	2.14	0.62
2:B:119:GLU:OE2	2:B:153:ARG:NH2	2.32	0.62
1:A:1238:A:N7	1:A:1303:C:H1'	2.14	0.62
1:A:562:C:C4	1:A:884:U:C5	2.88	0.62
4:D:190:ASP:HB2	4:D:192:GLU:HB3	1.80	0.62
1:A:9:G:H5'	5:E:122:GLU:OE2	1.99	0.62
1:A:720:C:H5'	18:R:52:PRO:HA	1.81	0.62
1:A:392:G:H2'	1:A:393:A:C8	2.34	0.62
1:A:292:G:H1	1:A:308:C:H42	1.47	0.62
1:A:116:A:N1	1:A:314:C:H1'	2.15	0.62
1:A:728:A:H2'	1:A:729:A:C8	2.35	0.62
3:C:150:LYS:HE2	3:C:167:TRP:HZ3	1.64	0.62
13:M:10:PRO:HB2	13:M:13:LYS:HD3	1.82	0.62
1:A:752:G:H4'	1:A:754:C:H5	1.64	0.62
2:B:100:GLY:C	2:B:102:LEU:H	1.98	0.62
1:A:1055:A:H2'	3:C:156:ARG:HD2	1.82	0.62
1:A:1503:A:OP1	1:A:1531:A:O2'	2.17	0.62
1:A:1314:C:H2'	1:A:1315:U:C6	2.35	0.62
7:G:34:GLY:O	7:G:36:LYS:N	2.33	0.62
18:R:53:ARG:HH11	18:R:53:ARG:HG2	1.65	0.61
1:A:974:A:P	14:N:41:ARG:HH21	2.22	0.61
11:K:91:ARG:HH11	11:K:92:GLU:HG3	1.65	0.61
15:O:4:THR:N	15:O:7:GLU:OE1	2.31	0.61
1:A:872:A:H4'	1:A:873:A:OP1	2.00	0.61
6:F:22:GLU:O	6:F:25:ILE:HG13	2.01	0.61
2:B:13:ALA:HA	2:B:209:ARG:HE	1.63	0.61
3:C:22:TRP:CZ3	3:C:32:LEU:HB3	2.35	0.61
2:B:180:LEU:O	2:B:182:ILE:N	2.33	0.61
1:A:1298:C:H5	7:G:114:ARG:HD3	1.64	0.61
3:C:83:ARG:HD2	3:C:87:LEU:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:49:THR:O	13:M:53:VAL:HG23	2.00	0.61
1:A:1010:G:O6	1:A:1019:C:N4	2.31	0.61
1:A:17:U:O4'	1:A:1080:A:H1'	2.00	0.61
8:H:120:THR:O	8:H:124:ALA:N	2.30	0.61
1:A:673:G:H5"	6:F:87:ARG:NH1	2.15	0.61
4:D:14:ARG:HA	4:D:39:PRO:HB3	1.82	0.61
1:A:1178:G:N2	1:A:1181:G:OP2	2.33	0.61
5:E:90:VAL:O	5:E:91:LEU:HD23	2.00	0.61
1:A:834:C:O5'	1:A:834:C:H6	1.83	0.61
1:A:316:G:OP2	1:A:351:G:O2'	2.19	0.61
6:F:18:GLN:HA	6:F:21:LEU:HD23	1.82	0.61
1:A:1454:G:H2'	1:A:1455:G:H8	1.65	0.61
19:S:28:LYS:HE3	19:S:47:HIS:CE1	2.35	0.61
1:A:1441:G:H4'	1:A:1443:G:OP1	2.00	0.61
1:A:975:A:O2'	14:N:32:SER:OG	2.19	0.61
2:B:74:LYS:NZ	2:B:166:ASP:OD2	2.25	0.61
1:A:640:A:N3	8:H:115:SER:OG	2.28	0.61
1:A:1074:G:OP1	5:E:64:ARG:NH1	2.34	0.61
18:R:58:LEU:HD22	18:R:62:GLU:OE1	2.01	0.61
1:A:92:C:H2'	1:A:93:G:C8	2.35	0.61
1:A:1214:C:O2'	1:A:1215:G:H5'	2.01	0.61
4:D:10:ARG:HG2	4:D:11:LEU:HD23	1.82	0.60
17:Q:7:THR:O	17:Q:23:VAL:HG13	2.01	0.60
1:A:707:C:OP1	11:K:85:ARG:NH1	2.29	0.60
5:E:39:GLY:H	5:E:71:LEU:HD12	1.64	0.60
1:A:1372:U:OP2	9:I:11:LYS:NZ	2.22	0.60
5:E:102:ALA:HB1	5:E:106:PRO:HB2	1.83	0.60
6:F:61:LEU:HB2	6:F:63:TYR:HE2	1.65	0.60
7:G:105:VAL:O	7:G:108:ALA:N	2.34	0.60
1:A:719:C:O2	18:R:50:ILE:HG13	2.01	0.60
1:A:398:C:H2'	1:A:399:G:C8	2.33	0.60
1:A:642:A:N3	8:H:113:SER:OG	2.33	0.60
1:A:382:A:H2'	1:A:383:A:C8	2.34	0.60
5:E:78:HIS:HB3	8:H:107:LEU:HD12	1.83	0.60
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.83	0.60
2:B:84:GLU:O	2:B:219:VAL:HG21	2.01	0.60
2:B:166:ASP:OD1	2:B:169:LYS:N	2.33	0.60
10:J:40:LEU:HD22	10:J:41:PRO:HD2	1.83	0.60
1:A:396:G:O2'	1:A:398:C:OP1	2.17	0.60
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.30	0.60
1:A:204:U:H4'	1:A:216:G:H5"	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:G:H2'	1:A:410:G:C8	2.34	0.60
13:M:15:VAL:O	13:M:19:LEU:HD12	2.01	0.60
12:L:102:ARG:HH21	12:L:108:ALA:HB3	1.66	0.60
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.37	0.60
4:D:68:TYR:OH	4:D:98:GLU:OE2	2.16	0.60
1:A:376:G:H5"	16:P:5:ARG:HD2	1.81	0.60
1:A:291:C:H41	1:A:305:G:HO2'	1.47	0.60
2:B:5:ILE:HD11	2:B:213:LEU:HD21	1.84	0.60
1:A:17:U:H2'	1:A:18:C:C6	2.35	0.60
17:Q:29:HIS:HB3	17:Q:33:GLY:N	2.08	0.60
1:A:1268:A:H2'	1:A:1269:A:C8	2.37	0.60
1:A:291:C:H3'	1:A:305:G:H22	1.67	0.60
1:A:1199:U:H4'	10:J:54:PHE:CE2	2.37	0.60
7:G:90:GLU:HG2	7:G:91:VAL:H	1.66	0.60
1:A:253:U:H2'	1:A:254:G:C8	2.36	0.60
1:A:959:A:O2'	1:A:984:C:O2'	2.10	0.60
1:A:408:A:H5'	4:D:116:GLN:HB2	1.84	0.60
4:D:10:ARG:HG3	4:D:40:PRO:HG3	1.83	0.60
1:A:678:U:O2	1:A:777:A:O2'	2.20	0.60
5:E:76:ILE:O	5:E:93:PRO:HB3	2.01	0.60
1:A:655:A:C2	1:A:754:C:N3	2.70	0.60
5:E:33:VAL:O	5:E:34:VAL:HG23	2.02	0.60
1:A:878:G:H2'	1:A:879:C:C6	2.35	0.59
1:A:1151:A:C2	1:A:1152:A:C5	2.90	0.59
1:A:392:G:H2'	1:A:393:A:H8	1.67	0.59
5:E:99:GLY:HA2	5:E:116:THR:O	2.01	0.59
1:A:1238:A:C8	1:A:1303:C:H1'	2.37	0.59
1:A:1518:A:H2'	1:A:1519:A:H8	1.67	0.59
13:M:59:TYR:O	13:M:63:THR:OG1	2.19	0.59
14:N:3:ARG:HE	14:N:6:LEU:HD12	1.66	0.59
1:A:670:G:N2	1:A:736:C:O2	2.29	0.59
2:B:178:ARG:HB3	8:H:72:PRO:HB3	1.84	0.59
1:A:291:C:N4	1:A:305:G:O2'	2.22	0.59
16:P:40:ASP:HB3	16:P:48:TRP:HB2	1.84	0.59
5:E:9:LYS:HB2	5:E:112:LEU:HD11	1.85	0.59
1:A:1435:G:H1	1:A:1466:C:H42	1.49	0.59
1:A:110:C:O2'	16:P:25:ARG:O	2.19	0.59
4:D:33:MET:SD	4:D:37:PRO:HA	2.42	0.59
1:A:521:G:OP2	12:L:54:LYS:NZ	2.25	0.59
1:A:737:A:H2'	1:A:738:C:H6	1.64	0.59
2:B:17:PHE:O	2:B:204:ASN:ND2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:ARG:HA	3:C:86:VAL:HG23	1.83	0.59
15:O:62:GLN:O	15:O:66:LEU:HD12	2.02	0.59
1:A:361:G:H2'	1:A:362:G:O4'	2.03	0.59
3:C:166:GLU:O	3:C:167:TRP:HB3	2.03	0.59
1:A:1077:G:H22	1:A:1079:G:H3'	1.66	0.59
2:B:177:ALA:HB1	2:B:182:ILE:HB	1.84	0.59
15:O:29:VAL:O	15:O:33:THR:OG1	2.21	0.59
1:A:1342:C:H2'	1:A:1343:G:C8	2.37	0.59
4:D:66:ARG:O	4:D:69:GLY:N	2.30	0.59
18:R:36:ASN:HB3	18:R:40:LEU:HD21	1.84	0.59
1:A:1370:G:H5'	9:I:12:GLU:HG3	1.85	0.59
1:A:1394:A:N7	1:A:1501:C:H4'	2.18	0.59
1:A:577:G:H1'	1:A:816:A:C4	2.37	0.59
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.38	0.59
1:A:794:A:C5	1:A:795:C:C5	2.90	0.59
1:A:1147:C:O2	9:I:16:ARG:NH1	2.36	0.59
3:C:74:GLY:HA2	3:C:77:ILE:HB	1.84	0.59
4:D:18:LYS:NZ	4:D:31:CYS:HB3	2.16	0.59
1:A:561:U:O2'	1:A:562:C:OP2	2.12	0.59
11:K:91:ARG:NH1	11:K:92:GLU:HG3	2.18	0.59
1:A:292:G:N2	1:A:309:G:C4	2.70	0.59
1:A:539:A:H2'	1:A:540:G:C8	2.38	0.59
1:A:1001:A:H2'	1:A:1002:G:C8	2.38	0.59
1:A:1148:U:H2'	1:A:1149:C:O4'	2.03	0.58
2:B:149:LEU:O	2:B:151:GLY:N	2.36	0.58
1:A:1228:C:H2'	1:A:1229:A:H8	1.68	0.58
1:A:688:G:O2'	1:A:704:A:N1	2.33	0.58
9:I:42:ARG:NH2	9:I:75:ASP:OD2	2.36	0.58
1:A:1071:C:H2'	1:A:1072:G:C8	2.34	0.58
6:F:66:GLU:O	6:F:67:MET:HB2	2.02	0.58
1:A:765:G:C2	1:A:812:C:H1'	2.38	0.58
1:A:1350:A:H61	1:A:1372:U:H3	1.49	0.58
10:J:63:PHE:HZ	14:N:45:ARG:HG3	1.68	0.58
8:H:85:ARG:HH12	8:H:134:ILE:HG23	1.68	0.58
19:S:39:THR:HG23	19:S:70:LYS:HD3	1.84	0.58
9:I:34:ASN:N	9:I:34:ASN:OD1	2.36	0.58
1:A:1081:G:OP1	5:E:18:ARG:HG3	2.03	0.58
19:S:30:LEU:HD11	19:S:50:ALA:HB2	1.84	0.58
1:A:193:C:H4'	20:T:61:SER:HB2	1.84	0.58
1:A:1385:G:H2'	1:A:1386:G:O4'	2.02	0.58
1:A:1119:C:H2'	1:A:1120:G:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:G:C2	1:A:309:G:C2	2.92	0.58
1:A:109:A:N7	1:A:326:G:C4	2.71	0.58
13:M:12:ASN:HA	13:M:46:LYS:HD3	1.84	0.58
1:A:190(J):U:H2'	1:A:190(K):G:H8	1.68	0.58
1:A:739:C:C6	1:A:739:C:H3'	2.39	0.58
1:A:727:G:P	1:A:742:G:H21	2.26	0.58
1:A:1070:U:H2'	1:A:1071:C:C6	2.38	0.58
1:A:532:A:N6	3:C:193:TYR:HB3	2.19	0.58
1:A:651:C:C2	1:A:652:U:C5	2.91	0.58
1:A:1061:G:H1	1:A:1195:C:H42	1.52	0.58
11:K:33:THR:HA	11:K:40:ILE:HG13	1.85	0.58
7:G:25:ALA:O	7:G:29:LYS:HB2	2.03	0.58
2:B:16:HIS:CE1	2:B:17:PHE:HD1	2.21	0.58
8:H:6:ILE:HG21	8:H:85:ARG:NH1	2.19	0.58
1:A:1203:C:H2'	1:A:1204:A:H8	1.67	0.58
6:F:2:ARG:HD3	6:F:92:LYS:HZ2	1.68	0.58
1:A:408:A:C6	1:A:409:G:N7	2.72	0.58
1:A:375:U:H3	1:A:389:A:H61	1.52	0.58
4:D:104:VAL:HG21	4:D:140:VAL:HG21	1.86	0.58
1:A:1183:A:O2'	1:A:1184:G:OP1	2.21	0.58
1:A:640:A:O2'	8:H:115:SER:HB3	2.04	0.58
18:R:31:LEU:HD22	18:R:66:LEU:HD12	1.85	0.58
18:R:65:ILE:C	18:R:67:ALA:H	2.07	0.58
1:A:1405:G:H2'	1:A:1406:U:C6	2.38	0.58
18:R:76:LEU:HB2	18:R:78:LEU:HD12	1.85	0.57
8:H:97:VAL:HG23	8:H:98:LYS:HG2	1.86	0.57
1:A:190(L):U:H3	20:T:105:SER:HG	1.51	0.57
1:A:1051:C:H2'	1:A:1052:U:C6	2.39	0.57
4:D:18:LYS:HB3	4:D:20:TYR:CE2	2.38	0.57
1:A:725:G:N2	1:A:732:C:O2	2.33	0.57
1:A:70:G:H2'	1:A:73:C:O4'	2.04	0.57
5:E:94:ALA:HB2	5:E:119:LEU:HD12	1.84	0.57
1:A:289:G:H2'	1:A:290:C:C6	2.39	0.57
4:D:110:PHE:CD1	4:D:110:PHE:N	2.71	0.57
1:A:106:C:H2'	1:A:107:G:O4'	2.03	0.57
6:F:69:GLU:O	6:F:72:VAL:HG23	2.04	0.57
5:E:6:PHE:HE2	5:E:36:ASP:H	1.53	0.57
1:A:702:A:O2'	1:A:703:G:OP1	2.21	0.57
1:A:1301:U:H3'	1:A:1302:U:H5"	1.87	0.57
1:A:229:U:O2'	16:P:23:ASP:OD2	2.23	0.57
1:A:1367:C:H5'	10:J:60:ARG:NH2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:90:VAL:HG12	12:L:92:ASP:H	1.68	0.57
1:A:601:C:H2'	1:A:602:A:C8	2.39	0.57
10:J:90:LEU:H	10:J:91:PRO:CD	2.17	0.57
1:A:475:G:H2'	1:A:476:G:H8	1.69	0.57
1:A:1502:A:H3'	1:A:1503:A:H5"	1.85	0.57
4:D:79:PHE:CZ	4:D:204:ILE:HG23	2.38	0.57
1:A:253:U:H2'	1:A:254:G:H8	1.68	0.57
1:A:779:C:N3	1:A:803:G:N2	2.49	0.57
1:A:952:U:H2'	1:A:953:G:H8	1.69	0.57
6:F:70:ASP:N	6:F:70:ASP:OD1	2.23	0.57
1:A:304:U:H2'	1:A:305:G:H8	1.66	0.57
15:O:69:TYR:CE1	15:O:73:GLU:HG3	2.38	0.57
14:N:47:LEU:HB3	14:N:53:LEU:HD21	1.86	0.57
8:H:38:ILE:HG21	8:H:111:ILE:HD13	1.87	0.57
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.40	0.57
17:Q:10:VAL:HG13	17:Q:19:VAL:HG23	1.85	0.57
1:A:426:G:OP1	4:D:36:ARG:NH2	2.34	0.56
1:A:1434:A:H2'	1:A:1435:G:O4'	2.05	0.56
1:A:145:G:H1	1:A:177:C:H42	1.53	0.56
1:A:663:A:N3	1:A:664:G:C8	2.73	0.56
1:A:678:U:H3	1:A:713:G:H22	1.52	0.56
18:R:36:ASN:O	18:R:38:GLU:N	2.38	0.56
1:A:1415:G:H2'	1:A:1416:G:C8	2.41	0.56
3:C:130:VAL:HG11	3:C:157:ILE:CG2	2.35	0.56
4:D:121:VAL:O	4:D:134:ASP:HA	2.06	0.56
1:A:49:U:H3	1:A:362:G:H1'	1.70	0.56
11:K:34:ASP:O	11:K:36:ASP:N	2.39	0.56
5:E:29:GLY:HA2	5:E:46:GLY:O	2.05	0.56
1:A:968:A:H4'	1:A:969:A:OP2	2.04	0.56
1:A:707:C:H2'	1:A:708:C:C6	2.40	0.56
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.39	0.56
10:J:46:ARG:HG2	10:J:64:GLU:HB3	1.88	0.56
1:A:1007:C:H2'	1:A:1008:C:C6	2.40	0.56
1:A:1347:G:O5'	9:I:107:ARG:HG2	2.05	0.56
6:F:74:ASP:O	6:F:77:ARG:HG2	2.06	0.56
3:C:20:SER:OG	3:C:40:ARG:NH2	2.39	0.56
1:A:137:C:H42	1:A:226:G:H1	1.52	0.56
1:A:509:A:N7	1:A:510:A:N6	2.53	0.56
5:E:110:LEU:O	5:E:115:VAL:HG23	2.05	0.56
1:A:560:U:C5'	1:A:561:U:H5"	2.35	0.56
1:A:546:G:OP2	4:D:72:GLU:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:A:H2'	1:A:301:G:O4'	2.05	0.56
10:J:37:PRO:HA	10:J:72:VAL:HG22	1.88	0.56
20:T:30:LYS:O	20:T:33:ILE:N	2.39	0.56
1:A:662:G:H2'	1:A:663:A:H8	1.69	0.56
18:R:53:ARG:NH1	18:R:58:LEU:O	2.38	0.56
15:O:25:THR:O	15:O:29:VAL:HG23	2.06	0.56
1:A:292:G:N2	1:A:309:G:N3	2.54	0.56
1:A:1358:U:H5"	1:A:1359:C:OP2	2.05	0.56
1:A:418:C:H2'	1:A:419:C:C6	2.40	0.56
3:C:35:GLU:O	3:C:39:ILE:HG13	2.06	0.56
1:A:541:G:O2'	4:D:42:GLN:N	2.39	0.56
1:A:1112:C:H1'	3:C:179:ARG:HD3	1.87	0.56
6:F:4:TYR:CE1	6:F:72:VAL:HG21	2.41	0.56
3:C:22:TRP:HB2	3:C:23:TYR:O	2.06	0.56
2:B:141:GLU:O	2:B:145:LEU:HD23	2.05	0.56
1:A:1432:G:N2	1:A:1469:G:O6	2.39	0.56
1:A:719:C:H3'	1:A:720:C:C5	2.41	0.55
5:E:110:LEU:HD22	5:E:115:VAL:HG21	1.88	0.55
1:A:1129:C:O4'	1:A:1146:A:N6	2.34	0.55
2:B:74:LYS:O	2:B:76:GLN:N	2.39	0.55
1:A:880:C:H5"	12:L:12:ARG:NH2	2.21	0.55
10:J:63:PHE:CZ	14:N:45:ARG:HG3	2.42	0.55
2:B:137:ARG:HH21	2:B:138:LEU:HD22	1.71	0.55
4:D:127:THR:HA	4:D:131:ARG:O	2.06	0.55
1:A:599:C:O2'	8:H:130:GLY:N	2.29	0.55
1:A:664:G:N2	1:A:666:G:C8	2.75	0.55
1:A:509:A:H62	1:A:510:A:H61	1.55	0.55
4:D:105:VAL:O	4:D:107:ARG:N	2.40	0.55
1:A:242:C:C2	1:A:285:G:N2	2.74	0.55
17:Q:41:LYS:NZ	17:Q:88:TYR:OH	2.38	0.55
1:A:1413:A:H2	1:A:1487:G:H22	1.54	0.55
3:C:43:LEU:HD21	3:C:68:VAL:HG21	1.89	0.55
1:A:95:U:H2'	1:A:96:G:H8	1.66	0.55
1:A:986:A:H1'	19:S:54:GLY:O	2.05	0.55
1:A:1070:U:OP1	5:E:18:ARG:NH2	2.38	0.55
5:E:131:ILE:O	5:E:135:THR:OG1	2.25	0.55
4:D:38:TYR:HB2	4:D:44:GLY:O	2.07	0.55
1:A:594:G:N2	1:A:646:U:H1'	2.22	0.55
1:A:1268:A:N3	1:A:1326:C:O2'	2.38	0.55
5:E:9:LYS:H	5:E:112:LEU:HD11	1.71	0.55
6:F:97:PHE:HB2	18:R:32:ARG:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:83:GLU:HA	10:J:86:MET:HE2	1.87	0.55
8:H:10:LEU:HA	8:H:13:ILE:HD11	1.89	0.55
15:O:18:PHE:CD2	15:O:21:ASP:HB2	2.41	0.55
9:I:93:ARG:HB2	9:I:93:ARG:HH11	1.72	0.55
1:A:1402:C:H2'	1:A:1403:C:H6	1.71	0.55
5:E:12:LEU:HG	5:E:13:ILE:N	2.20	0.55
2:B:185:ILE:HA	2:B:199:TYR:O	2.06	0.55
1:A:149:A:H2'	1:A:150:C:C6	2.41	0.55
8:H:10:LEU:HD23	8:H:13:ILE:HD11	1.89	0.55
6:F:78:GLU:HB3	6:F:79:LEU:HD23	1.88	0.55
11:K:27:ASN:OD1	11:K:28:THR:N	2.37	0.55
21:V:6:ARG:HH11	21:V:15:ARG:NE	2.05	0.55
13:M:16:ASP:HB2	13:M:31:LYS:HE2	1.87	0.55
1:A:1173:G:H2'	1:A:1174:G:H8	1.72	0.55
1:A:455:C:H42	1:A:477:G:H1	1.54	0.55
1:A:1060:C:C5	3:C:2:GLY:HA3	2.37	0.55
1:A:372:C:H4'	1:A:373:A:OP1	2.07	0.55
15:O:11:VAL:HG21	15:O:34:LEU:HD22	1.87	0.55
1:A:691:G:O2'	1:A:797:C:H4'	2.07	0.55
1:A:869:G:H4'	1:A:872:A:N7	2.21	0.55
1:A:518:C:O3'	12:L:50:SER:OG	2.24	0.55
15:O:33:THR:HA	15:O:36:ILE:HD12	1.87	0.55
1:A:1485:U:H2'	1:A:1486:G:H8	1.72	0.55
4:D:152:SER:O	4:D:155:LEU:HB2	2.07	0.55
4:D:131:ARG:HG2	4:D:132:ARG:H	1.71	0.55
11:K:24:SER:OG	11:K:25:TYR:N	2.39	0.55
1:A:1116:C:O2'	9:I:108:VAL:HG11	2.06	0.55
1:A:517:G:H1	1:A:533:A:P	2.30	0.54
3:C:3:ASN:N	3:C:3:ASN:OD1	2.40	0.54
1:A:310:G:H2'	1:A:311:C:H6	1.70	0.54
15:O:4:THR:O	15:O:7:GLU:HG3	2.06	0.54
1:A:1513:A:H2'	1:A:1514:C:C6	2.42	0.54
8:H:67:PRO:O	8:H:76:PRO:HG3	2.07	0.54
1:A:804:U:H5"	1:A:805:C:OP2	2.07	0.54
5:E:107:ARG:HG2	5:E:107:ARG:HH11	1.72	0.54
1:A:1488:G:H2'	1:A:1489:G:H8	1.72	0.54
6:F:100:ASN:OD1	6:F:100:ASN:N	2.40	0.54
1:A:1378:C:H5"	7:G:6:ARG:HD3	1.89	0.54
1:A:427:U:OP2	1:A:428:G:O2'	2.15	0.54
1:A:501:C:O3'	12:L:118:SER:OG	2.25	0.54
10:J:78:ASN:HB3	10:J:80:LYS:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:A:H2'	1:A:716:A:C8	2.43	0.54
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.42	0.54
18:R:73:ALA:O	18:R:79:LEU:HB2	2.07	0.54
1:A:294:U:H2'	1:A:295:C:C6	2.41	0.54
5:E:139:LEU:HD23	5:E:142:LEU:HD21	1.88	0.54
1:A:673:G:H5'	6:F:87:ARG:HD3	1.88	0.54
1:A:1152:A:H5'	10:J:13:HIS:CB	2.36	0.54
1:A:745:C:H1'	1:A:836:G:O2'	2.08	0.54
1:A:1044:A:H5'	1:A:1045:C:OP2	2.08	0.54
1:A:294:U:H2'	1:A:295:C:H6	1.73	0.54
1:A:67:C:H2'	1:A:68:G:H8	1.71	0.54
1:A:779:C:H2'	1:A:780:A:O4'	2.07	0.54
1:A:673:G:C5'	6:F:87:ARG:HD3	2.38	0.54
2:B:163:PHE:HA	2:B:185:ILE:O	2.07	0.54
8:H:6:ILE:HD11	8:H:31:PHE:CD2	2.43	0.54
1:A:727:G:OP1	1:A:742:G:N2	2.31	0.54
3:C:40:ARG:HH11	3:C:55:VAL:HB	1.73	0.54
1:A:10:A:H2'	1:A:11:G:C8	2.38	0.54
10:J:61:GLU:OE1	14:N:45:ARG:HD2	2.08	0.54
1:A:1007:C:H2'	1:A:1008:C:H6	1.72	0.54
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.25	0.54
1:A:1199:U:H4'	10:J:54:PHE:HE2	1.72	0.54
1:A:562:C:H4'	1:A:563:A:O5'	2.08	0.54
1:A:1298:C:H4'	1:A:1299:A:O4'	2.08	0.54
1:A:445:G:H2'	1:A:446:G:H8	1.71	0.54
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.89	0.54
1:A:927:G:H1	1:A:1390:U:H3	1.54	0.54
1:A:18:C:OP1	5:E:127:ASN:ND2	2.41	0.54
8:H:17:THR:HA	8:H:65:TYR:OH	2.06	0.54
8:H:44:PHE:HA	8:H:79:VAL:HG12	1.90	0.54
1:A:418:C:H2'	1:A:419:C:H6	1.71	0.54
1:A:76:C:H2'	1:A:77:G:H8	1.73	0.54
4:D:10:ARG:HG2	4:D:11:LEU:CD2	2.38	0.54
6:F:52:ILE:O	6:F:55:ASP:HB2	2.08	0.54
13:M:29:ARG:HD3	13:M:64:TRP:CD1	2.43	0.54
17:Q:13:ASP:HB2	17:Q:53:LEU:HB2	1.88	0.54
1:A:163:C:H2'	1:A:164:U:C6	2.43	0.54
14:N:27:CYS:SG	14:N:43:CYS:SG	3.06	0.54
16:P:14:ASN:ND2	16:P:14:ASN:O	2.40	0.54
1:A:337:C:H2'	1:A:338:A:C8	2.43	0.53
4:D:53:ASP:OD2	5:E:107:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:29:ARG:HD3	13:M:64:TRP:NE1	2.22	0.53
20:T:26:ASN:OD1	20:T:71:THR:HG23	2.08	0.53
15:O:28:GLN:HA	15:O:31:LEU:HD12	1.90	0.53
1:A:676:A:H2'	1:A:677:U:H6	1.72	0.53
1:A:594:G:H22	1:A:646:U:H1'	1.72	0.53
1:A:375:U:H2'	1:A:376:G:H8	1.73	0.53
1:A:1343:G:H2'	1:A:1344:C:C6	2.44	0.53
16:P:77:ALA:HB3	16:P:79:VAL:HG23	1.90	0.53
6:F:13:ASN:N	6:F:13:ASN:OD1	2.41	0.53
1:A:514:C:O2	1:A:538:G:N2	2.41	0.53
1:A:632:A:C8	1:A:633:G:C8	2.97	0.53
1:A:1361(A):C:O2'	1:A:1362:C:H5'	2.07	0.53
2:B:149:LEU:HD23	2:B:152:PHE:HD2	1.73	0.53
3:C:152:ILE:HD13	3:C:201:TYR:CE1	2.42	0.53
18:R:36:ASN:O	18:R:36:ASN:ND2	2.29	0.53
19:S:10:PHE:O	19:S:39:THR:OG1	2.25	0.53
1:A:1003(A):G:N2	1:A:1037:C:O2	2.36	0.53
13:M:4:ILE:HD11	13:M:9:ILE:HG21	1.90	0.53
1:A:872:A:C2	1:A:874:G:C5	2.97	0.53
1:A:736:C:H2'	1:A:737:A:H8	1.73	0.53
1:A:678:U:H3	1:A:713:G:N2	2.07	0.53
4:D:110:PHE:HD1	4:D:110:PHE:N	2.06	0.53
2:B:133:LYS:O	2:B:137:ARG:HB2	2.08	0.53
1:A:1257:U:H5"	1:A:1258:G:OP2	2.09	0.53
12:L:57:LYS:HA	12:L:67:THR:HA	1.91	0.53
1:A:8:A:H5"	5:E:120:THR:O	2.08	0.53
1:A:765:G:H22	1:A:812:C:H1'	1.71	0.53
4:D:43:HIS:O	4:D:45:GLN:N	2.42	0.53
1:A:625:G:H2'	1:A:626:U:C6	2.43	0.53
1:A:564:C:H5'	17:Q:32:TYR:CE2	2.43	0.53
1:A:114:U:H2'	1:A:115:G:C8	2.43	0.53
3:C:9:GLY:HA2	3:C:12:LEU:HD21	1.90	0.53
1:A:6:G:H2'	5:E:119:LEU:HD21	1.90	0.53
1:A:1356:G:H2'	1:A:1357:A:C8	2.43	0.53
1:A:556:C:H2'	1:A:557:G:H8	1.74	0.53
1:A:1015:A:N3	1:A:1218:C:O2'	2.39	0.53
1:A:410:G:H2'	1:A:429:U:C5	2.44	0.53
1:A:831:U:OP2	2:B:21:ARG:NH1	2.41	0.53
7:G:138:LYS:HD3	7:G:139:GLU:HG3	1.91	0.53
1:A:1518:A:H2'	1:A:1519:A:C8	2.43	0.53
17:Q:21:VAL:O	17:Q:41:LYS:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.74	0.53
7:G:95:ARG:NH1	7:G:99:LEU:HD11	2.24	0.53
15:O:57:LEU:HD23	15:O:60:VAL:HB	1.89	0.53
1:A:516:U:C5	1:A:517:G:C6	2.97	0.53
1:A:1386:G:O2'	1:A:1387:G:H5'	2.09	0.53
14:N:24:CYS:HB3	14:N:28:GLY:H	1.74	0.53
1:A:588:G:H21	1:A:653:A:H2	1.57	0.53
1:A:1081:G:H2'	1:A:1082:G:H8	1.74	0.53
1:A:1507:A:C2	1:A:1508:G:C4	2.97	0.53
5:E:100:VAL:HA	5:E:118:ILE:HG22	1.91	0.53
1:A:1014:A:H2'	1:A:1015:A:C8	2.44	0.53
10:J:8:LEU:HD12	10:J:20:ALA:HB2	1.90	0.53
1:A:512:U:H2'	1:A:513:C:C6	2.44	0.53
4:D:120:LEU:O	4:D:125:HIS:HB2	2.09	0.53
6:F:54:LYS:O	6:F:56:PRO:HD3	2.09	0.53
1:A:1499:A:H2'	1:A:1500:A:H8	1.73	0.53
12:L:32:PHE:HA	12:L:85:ILE:O	2.09	0.53
10:J:19:SER:OG	10:J:91:PRO:HG3	2.08	0.53
6:F:100:ASN:HA	18:R:28:GLU:HA	1.91	0.53
4:D:57:ARG:NH2	4:D:205:GLU:OE2	2.28	0.53
1:A:262:A:H4'	20:T:75:ASN:HB2	1.90	0.53
14:N:23:ARG:HG3	14:N:30:ALA:HB2	1.91	0.52
3:C:119:ARG:O	3:C:123:GLN:HG3	2.08	0.52
12:L:69:TYR:O	12:L:100:ILE:HG13	2.09	0.52
12:L:69:TYR:HB3	12:L:99:HIS:CD2	2.44	0.52
3:C:19:GLU:HB3	3:C:40:ARG:HH12	1.74	0.52
3:C:152:ILE:HD13	3:C:201:TYR:HE1	1.74	0.52
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.90	0.52
1:A:1099:G:H5"	1:A:1100:C:OP2	2.10	0.52
3:C:22:TRP:N	3:C:22:TRP:CD1	2.77	0.52
6:F:82:ARG:HD2	6:F:82:ARG:N	2.20	0.52
1:A:501:C:H1'	1:A:549:C:H1'	1.91	0.52
3:C:173:VAL:O	3:C:173:VAL:HG12	2.08	0.52
1:A:563:A:N7	1:A:567:G:H1'	2.24	0.52
1:A:983:A:H5"	1:A:984:C:OP2	2.09	0.52
15:O:61:GLY:O	15:O:64:ARG:N	2.42	0.52
1:A:819:A:H4'	1:A:820:U:OP2	2.09	0.52
1:A:1093:A:N3	1:A:1095:U:H5'	2.24	0.52
5:E:99:GLY:O	5:E:101:ILE:N	2.42	0.52
6:F:22:GLU:O	6:F:24:GLU:N	2.42	0.52
13:M:33:ALA:HB2	13:M:64:TRP:HH2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:C:C2'	1:A:1076:C:H5'	2.40	0.52
5:E:32:VAL:HG11	5:E:59:GLY:HA2	1.92	0.52
1:A:667:G:C2	1:A:740:U:O2	2.62	0.52
4:D:43:HIS:HA	4:D:46:LYS:HE3	1.91	0.52
6:F:62:TRP:CZ2	6:F:64:GLN:HB2	2.44	0.52
6:F:11:ASN:HB2	6:F:13:ASN:OD1	2.10	0.52
1:A:161:A:N1	1:A:347:G:O2'	2.43	0.52
1:A:872:A:C2	1:A:874:G:C4	2.97	0.52
1:A:426:G:H2'	1:A:427:U:C6	2.45	0.52
2:B:93:VAL:HG11	2:B:97:TRP:HE3	1.74	0.52
11:K:17:GLY:O	11:K:80:VAL:HA	2.10	0.52
1:A:243:A:N6	1:A:281:G:O2'	2.43	0.52
1:A:355:C:C4	1:A:356:A:N7	2.77	0.52
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.10	0.52
8:H:12:ARG:HD3	8:H:26:VAL:HG22	1.91	0.52
1:A:657:G:N2	1:A:749:C:N3	2.52	0.52
15:O:42:HIS:CE1	15:O:46:HIS:HD2	2.28	0.52
1:A:1073:U:OP1	5:E:57:LYS:HD2	2.08	0.52
1:A:428:G:C5	1:A:430:A:C6	2.98	0.52
1:A:676:A:H2'	1:A:677:U:C6	2.45	0.52
1:A:979:C:H42	14:N:18:VAL:HB	1.75	0.52
12:L:102:ARG:HD3	12:L:110:VAL:HG22	1.92	0.52
1:A:222:U:H2'	1:A:223:U:C6	2.45	0.52
21:V:6:ARG:HD2	21:V:15:ARG:HH21	1.74	0.52
18:R:59:SER:OG	18:R:60:ALA:N	2.43	0.52
12:L:113:ARG:NH2	12:L:116:SER:HB2	2.23	0.52
1:A:973:G:O3'	14:N:41:ARG:NH2	2.40	0.52
1:A:1367:C:N3	1:A:1368:G:C8	2.77	0.52
1:A:397:A:H5"	1:A:397:A:N3	2.24	0.52
20:T:81:LYS:O	20:T:85:MET:HB2	2.10	0.52
1:A:1206:G:H4'	3:C:192:THR:O	2.09	0.51
1:A:1119:C:OP2	9:I:9:ARG:NH2	2.43	0.51
1:A:64:G:H4'	1:A:65:U:H3'	1.91	0.51
17:Q:25:ARG:HH11	17:Q:27:PHE:HE2	1.57	0.51
1:A:1086:U:H3	1:A:1099:G:H22	1.58	0.51
1:A:1500:A:H5"	1:A:1508:G:H5"	1.92	0.51
1:A:973:G:H1'	10:J:54:PHE:CE1	2.45	0.51
20:T:43:LEU:HD22	20:T:48:LYS:HG3	1.92	0.51
1:A:1516:G:N2	1:A:1520:G:N3	2.59	0.51
5:E:155:GLU:HG2	5:E:156:ALA:N	2.25	0.51
1:A:17:U:O2'	1:A:1079:G:O2'	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:75:HIS:HA	12:L:102:ARG:HH22	1.74	0.51
1:A:296:U:C2	1:A:297:G:C8	2.99	0.51
1:A:1314:C:OP2	19:S:4:SER:OG	2.28	0.51
1:A:1439:C:OP2	20:T:38:LYS:NZ	2.43	0.51
1:A:1379:G:O6	7:G:2:ALA:N	2.43	0.51
7:G:68:ASN:O	7:G:135:VAL:HG13	2.09	0.51
18:R:53:ARG:HG2	18:R:53:ARG:NH1	2.22	0.51
2:B:108:ILE:HG21	2:B:152:PHE:HE2	1.75	0.51
1:A:296:U:N3	1:A:297:G:N7	2.58	0.51
1:A:1058:G:H2'	1:A:1059:C:C6	2.45	0.51
1:A:204:U:H5"	1:A:216:G:O4'	2.10	0.51
11:K:109:VAL:HA	18:R:85:LEU:O	2.10	0.51
1:A:776:G:N2	1:A:802:A:OP2	2.44	0.51
1:A:583:A:H1'	1:A:759:A:N6	2.25	0.51
1:A:1415:G:H1	1:A:1485:U:H3	1.57	0.51
12:L:117:ARG:O	12:L:120:TYR:N	2.39	0.51
12:L:46:LYS:HB2	12:L:92:ASP:O	2.11	0.51
9:I:35:GLU:HA	9:I:38:GLN:NE2	2.24	0.51
3:C:172:ARG:C	3:C:174:PRO:HD3	2.31	0.51
1:A:1105:A:O2'	1:A:1106:G:H5'	2.10	0.51
1:A:599:C:HO2'	8:H:130:GLY:H	1.56	0.51
3:C:137:ALA:O	3:C:141:VAL:HG23	2.10	0.51
1:A:1039:C:H2'	1:A:1040:U:C6	2.46	0.51
1:A:325:A:OP2	20:T:70:SER:HB2	2.11	0.51
1:A:663:A:C4	1:A:664:G:C8	2.99	0.51
4:D:116:GLN:O	4:D:118:ARG:N	2.44	0.51
15:O:26:GLU:CG	15:O:81:LEU:HD22	2.41	0.51
8:H:111:ILE:HG13	8:H:135:CYS:SG	2.51	0.51
1:A:751:U:H2'	1:A:752:G:H5'	1.93	0.51
2:B:204:ASN:OD1	2:B:207:ALA:N	2.43	0.51
2:B:144:ARG:HD3	2:B:148:TYR:HE2	1.76	0.51
1:A:1527:C:C5	1:A:1528:U:H5	2.29	0.51
3:C:187:ALA:O	3:C:188:LEU:HB2	2.11	0.51
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.92	0.51
1:A:866:C:C5	1:A:867:G:H1'	2.46	0.51
6:F:9:VAL:HG22	6:F:60:PHE:CE1	2.46	0.51
2:B:69:LEU:HB3	2:B:162:ILE:HG22	1.92	0.51
8:H:104:ARG:HG3	8:H:104:ARG:HH11	1.76	0.51
1:A:1348:U:H2'	1:A:1349:A:H8	1.75	0.51
1:A:714:G:H21	1:A:777:A:H1'	1.76	0.51
1:A:807:A:H2'	1:A:808:C:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:G:H2'	1:A:928:G:H8	1.76	0.51
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.92	0.51
1:A:1346:A:N1	1:A:1374:A:H5"	2.25	0.51
3:C:46:GLU:O	3:C:48:TYR:N	2.40	0.51
18:R:34:TYR:CD2	18:R:34:TYR:N	2.78	0.51
1:A:1347:G:O2'	1:A:1348:U:OP2	2.28	0.51
4:D:100:ARG:NH1	4:D:137:SER:HA	2.26	0.51
4:D:104:VAL:HG11	4:D:146:ILE:HG13	1.92	0.51
16:P:30:GLY:O	16:P:32:TYR:N	2.43	0.51
1:A:1105:A:H2'	1:A:1106:G:C8	2.44	0.51
1:A:310:G:OP1	16:P:26:ARG:NH1	2.44	0.51
7:G:37:ASN:OD1	9:I:41:VAL:HG23	2.11	0.51
1:A:635:G:C6	1:A:636:U:C4	2.99	0.51
1:A:1460:A:H2'	1:A:1461:G:O4'	2.11	0.51
1:A:484:G:C8	1:A:486:U:C6	2.98	0.51
2:B:189:ASP:OD2	2:B:205:ASP:HB2	2.11	0.51
1:A:662:G:H2'	1:A:663:A:C8	2.45	0.51
1:A:826:C:O2'	1:A:827:U:H5'	2.11	0.51
2:B:178:ARG:HH21	8:H:74:PRO:HG3	1.76	0.51
1:A:744:C:H2'	1:A:745:C:H6	1.75	0.51
10:J:84:GLN:HA	10:J:87:THR:HG22	1.91	0.51
1:A:414:A:C2	1:A:415:A:C4	2.99	0.51
13:M:74:VAL:O	13:M:78:ILE:HG13	2.10	0.51
1:A:740:U:C6	1:A:740:U:H3'	2.46	0.51
1:A:721:G:OP2	18:R:53:ARG:HB2	2.09	0.51
1:A:1055:A:H62	1:A:1200:C:N4	2.03	0.51
1:A:1207:G:H2'	1:A:1208:C:C6	2.46	0.51
3:C:193:TYR:HE1	3:C:196:LEU:HD11	1.74	0.51
1:A:8:A:C6	4:D:209:ARG:HB2	2.46	0.51
1:A:296:U:C2	1:A:297:G:N7	2.79	0.51
1:A:952:U:H2'	1:A:953:G:C8	2.46	0.51
1:A:1057:G:H5"	3:C:154:SER:O	2.11	0.51
1:A:883:C:C2'	1:A:884:U:H5'	2.40	0.51
1:A:697:U:HO2'	1:A:785:G:HO2'	1.59	0.51
1:A:800:G:H2'	1:A:801:U:C5	2.46	0.51
1:A:753:A:H5'	1:A:754:C:C5	2.46	0.50
5:E:31:LEU:HD12	5:E:44:GLY:O	2.11	0.50
11:K:48:ILE:HG21	11:K:63:LEU:HD12	1.92	0.50
11:K:99:GLN:HG2	11:K:105:VAL:HG21	1.93	0.50
3:C:180:ALA:O	3:C:182:ILE:HD12	2.12	0.50
1:A:426:G:H2'	1:A:427:U:H6	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:81:ILE:HB	6:F:82:ARG:NH1	2.26	0.50
1:A:878:G:H5'	8:H:89:PRO:HG2	1.91	0.50
2:B:105:PHE:CG	2:B:158:LEU:HD21	2.46	0.50
4:D:200:GLU:O	4:D:204:ILE:HG13	2.10	0.50
3:C:132:ARG:HB3	3:C:136:GLN:HE22	1.76	0.50
1:A:563:A:C8	1:A:567:G:H1'	2.46	0.50
1:A:1318:A:H4'	19:S:10:PHE:CE2	2.46	0.50
17:Q:43:LEU:HB2	17:Q:68:ARG:O	2.11	0.50
2:B:167:PRO:HG2	2:B:192:SER:HB2	1.93	0.50
1:A:719:C:OP2	1:A:720:C:N4	2.36	0.50
15:O:37:ASN:HA	15:O:40:SER:OG	2.11	0.50
18:R:37:VAL:HG21	18:R:78:LEU:HB3	1.92	0.50
1:A:1053:G:C6	1:A:1199:U:C2	2.99	0.50
1:A:1198:G:H2'	1:A:1199:U:C6	2.46	0.50
6:F:10:LEU:O	6:F:59:TYR:HB3	2.11	0.50
10:J:81:THR:O	10:J:84:GLN:N	2.37	0.50
1:A:1348:U:O2'	9:I:120:ARG:HD2	2.11	0.50
1:A:759:A:H5"	1:A:881:G:H5'	1.94	0.50
20:T:86:ARG:HG2	20:T:90:GLN:NE2	2.26	0.50
3:C:182:ILE:HA	3:C:202:ILE:O	2.11	0.50
15:O:41:GLU:O	15:O:44:LYS:N	2.45	0.50
1:A:947:G:HO2'	1:A:1306:A:HO2'	1.59	0.50
4:D:70:ILE:HG12	4:D:100:ARG:NE	2.27	0.50
13:M:108:ARG:HH12	13:M:111:LYS:HE3	1.76	0.50
1:A:568:G:N2	1:A:883:C:C2	2.79	0.50
1:A:654:G:C6	1:A:753:A:C5	3.00	0.50
1:A:1378:C:OP2	7:G:6:ARG:HA	2.12	0.50
1:A:1107:C:O2	1:A:1191:A:O2'	2.24	0.50
8:H:46:LYS:HE2	8:H:63:LEU:O	2.11	0.50
1:A:875:C:H1'	8:H:15:ASN:ND2	2.26	0.50
8:H:37:ARG:NH2	8:H:118:VAL:O	2.43	0.50
6:F:37:VAL:HG11	6:F:40:VAL:HG23	1.93	0.50
1:A:731:G:OP1	1:A:766:A:H1'	2.11	0.50
18:R:65:ILE:O	18:R:67:ALA:N	2.45	0.50
1:A:146:G:H2'	1:A:147:G:H8	1.77	0.50
1:A:1337:G:H5"	1:A:1338:G:OP1	2.12	0.50
14:N:34:TYR:O	14:N:36:PHE:N	2.42	0.50
1:A:417:C:H42	1:A:426:G:H1	1.59	0.50
3:C:156:ARG:H	3:C:196:LEU:HD22	1.76	0.50
1:A:1417:G:O3'	1:A:1418:A:H8	1.93	0.50
17:Q:6:LEU:O	17:Q:58:GLU:HA	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:LEU:HD23	2:B:152:PHE:CD2	2.46	0.50
1:A:563:A:C8	1:A:567:G:C1'	2.95	0.50
5:E:139:LEU:HA	5:E:142:LEU:HG	1.94	0.50
1:A:859:A:H2'	1:A:860:A:O4'	2.12	0.50
1:A:458:C:H3'	1:A:459:G:C8	2.47	0.50
1:A:496:A:H4'	1:A:497:A:H5'	1.92	0.50
1:A:582:U:C2	1:A:760:G:C6	2.99	0.50
1:A:1416:G:H2'	1:A:1417:G:O4'	2.12	0.50
12:L:117:ARG:NH2	12:L:124:LYS:HD3	2.26	0.50
5:E:100:VAL:CG1	5:E:107:ARG:HG3	2.42	0.50
4:D:104:VAL:O	4:D:108:LEU:HB2	2.11	0.50
11:K:21:ILE:HG12	11:K:30:VAL:HG13	1.93	0.50
1:A:1402:C:C2	1:A:1403:C:C6	3.00	0.50
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.93	0.50
16:P:50:LYS:HG2	16:P:51:VAL:N	2.25	0.50
15:O:5:LYS:O	15:O:9:GLN:HG2	2.12	0.50
1:A:1132:C:H2'	1:A:1133:G:H8	1.76	0.50
1:A:1269:A:H2	1:A:1312:G:N3	2.09	0.50
1:A:1311:G:N2	1:A:1327:C:N3	2.60	0.50
1:A:66:G:N2	1:A:172:A:N3	2.60	0.50
2:B:74:LYS:HD2	2:B:166:ASP:HB2	1.92	0.50
12:L:41:ARG:HG2	12:L:42:THR:H	1.77	0.50
18:R:66:LEU:O	18:R:66:LEU:HD23	2.11	0.50
1:A:335:C:H2'	1:A:336:C:C6	2.47	0.50
20:T:37:SER:O	20:T:41:ILE:HG13	2.11	0.50
8:H:2:LEU:HD12	8:H:3:THR:H	1.77	0.50
1:A:719:C:O2'	18:R:49:LYS:HB3	2.12	0.49
1:A:1235:U:H2'	1:A:1236:A:O4'	2.11	0.49
10:J:38:ILE:HB	10:J:71:LEU:O	2.12	0.49
17:Q:92:ARG:HH11	17:Q:95:TYR:HE2	1.60	0.49
14:N:40:CYS:SG	14:N:41:ARG:N	2.85	0.49
1:A:136:C:H2'	1:A:137:C:H6	1.77	0.49
12:L:27:LEU:O	12:L:29:GLY:N	2.44	0.49
1:A:1391:U:H2'	1:A:1392:G:C8	2.47	0.49
1:A:730:G:N2	1:A:765:G:H5"	2.27	0.49
8:H:86:ILE:HD13	8:H:133:LEU:HG	1.93	0.49
5:E:52:PRO:HA	5:E:55:VAL:CG2	2.42	0.49
1:A:1045:C:H2'	1:A:1046:A:O4'	2.12	0.49
1:A:643:C:H5'	8:H:31:PHE:CE1	2.47	0.49
1:A:59:A:H1'	1:A:354:G:N2	2.27	0.49
12:L:124:LYS:HD2	12:L:125:PRO:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:100:VAL:HG12	5:E:107:ARG:HG3	1.93	0.49
5:E:76:ILE:HD12	5:E:118:ILE:HD11	1.95	0.49
1:A:360:A:H2'	1:A:361:G:O4'	2.12	0.49
1:A:1058:G:OP1	3:C:199:LYS:HE2	2.12	0.49
11:K:48:ILE:HD11	11:K:64:ALA:HA	1.94	0.49
1:A:1055:A:O2'	3:C:161:GLU:O	2.24	0.49
1:A:582:U:N3	1:A:760:G:C6	2.80	0.49
7:G:24:THR:O	7:G:27:ILE:N	2.45	0.49
2:B:101:MET:HA	2:B:108:ILE:HG13	1.93	0.49
4:D:18:LYS:HE2	4:D:31:CYS:SG	2.53	0.49
1:A:933:G:N2	1:A:935:A:O4'	2.46	0.49
1:A:1173:G:H2'	1:A:1174:G:C8	2.48	0.49
14:N:23:ARG:HG2	14:N:24:CYS:H	1.78	0.49
3:C:69:HIS:HA	3:C:104:GLN:O	2.11	0.49
1:A:126:G:OP1	1:A:605:U:O2'	2.23	0.49
1:A:878:G:C5	1:A:879:C:C5	3.01	0.49
8:H:89:PRO:HB3	8:H:92:ARG:HH22	1.78	0.49
1:A:1267:C:C5	1:A:1268:A:C5	3.01	0.49
1:A:291:C:H3'	1:A:305:G:N2	2.28	0.49
1:A:973:G:H1'	10:J:54:PHE:HE1	1.76	0.49
2:B:189:ASP:OD1	2:B:190:THR:N	2.45	0.49
20:T:29:LYS:NZ	20:T:66:ALA:HA	2.26	0.49
1:A:740:U:H3'	1:A:740:U:H6	1.77	0.49
1:A:542:G:H5'	4:D:41:GLY:HA3	1.93	0.49
4:D:96:LEU:O	4:D:97:LEU:HD23	2.12	0.49
8:H:38:ILE:HG22	8:H:39:LEU:HD23	1.93	0.49
1:A:598:U:H2'	1:A:599:C:H6	1.77	0.49
15:O:11:VAL:O	15:O:15:PHE:HB2	2.12	0.49
1:A:1217:C:H2'	1:A:1218:C:C6	2.48	0.49
3:C:138:VAL:HG13	3:C:149:ALA:HB3	1.95	0.49
1:A:458:C:H3'	1:A:459:G:H8	1.77	0.49
1:A:1157:A:C6	1:A:1180:A:C6	3.00	0.49
2:B:186:ALA:HB3	2:B:197:VAL:HG21	1.95	0.49
1:A:1386:G:H2'	1:A:1387:G:H8	1.77	0.49
20:T:59:ALA:O	20:T:63:ILE:HG12	2.12	0.49
2:B:168:THR:HG21	2:B:192:SER:HA	1.95	0.49
7:G:67:GLU:HA	7:G:70:LYS:HD2	1.94	0.49
1:A:720:C:H4'	18:R:63:GLN:NE2	2.26	0.49
1:A:869:G:O2'	1:A:872:A:N6	2.39	0.49
1:A:980:C:O2	14:N:19:ARG:HA	2.13	0.49
12:L:71:PRO:O	12:L:102:ARG:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.48	0.49
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.48	0.49
4:D:196:LEU:HB2	4:D:198:VAL:HG22	1.94	0.49
1:A:920:U:C2	1:A:921:U:C5	3.01	0.49
1:A:771:G:C2	1:A:809:G:N1	2.81	0.49
1:A:932:C:H4'	7:G:4:ARG:NH2	2.28	0.49
1:A:654:G:C6	1:A:753:A:C4	3.01	0.49
1:A:397:A:N6	1:A:548:G:C5	2.81	0.49
7:G:113:GLU:HB2	7:G:119:ARG:HG2	1.95	0.49
1:A:409:G:C4	1:A:410:G:C8	3.01	0.49
2:B:115:LEU:HD11	2:B:153:ARG:NH2	2.28	0.49
5:E:107:ARG:HH11	5:E:107:ARG:CG	2.25	0.49
8:H:9:MET:HG3	8:H:26:VAL:HG11	1.94	0.49
1:A:269:C:H2'	1:A:270:A:C8	2.48	0.49
1:A:1504:G:OP1	1:A:1507:A:H4'	2.12	0.49
1:A:831:U:H5'	2:B:22:LYS:CG	2.39	0.49
17:Q:7:THR:HG23	17:Q:58:GLU:CG	2.41	0.49
4:D:155:LEU:O	4:D:159:ARG:HG3	2.12	0.49
11:K:18:ARG:HG2	11:K:33:THR:OG1	2.13	0.49
1:A:303:A:H1'	1:A:555:C:O2'	2.13	0.49
1:A:1286:A:H2'	1:A:1287:A:H4'	1.95	0.49
1:A:664:G:H2'	1:A:666:G:OP1	2.12	0.48
8:H:121:ASP:HA	8:H:124:ALA:HB3	1.95	0.48
1:A:373:A:N3	1:A:373:A:H2'	2.27	0.48
2:B:178:ARG:NH2	8:H:74:PRO:HG3	2.27	0.48
1:A:103:C:HO2'	1:A:172:A:N6	2.10	0.48
1:A:993:G:H2'	1:A:995:C:H41	1.77	0.48
5:E:39:GLY:N	5:E:71:LEU:HD12	2.28	0.48
6:F:6:VAL:HB	6:F:63:TYR:HB2	1.95	0.48
1:A:1435:G:H1	1:A:1466:C:N4	2.11	0.48
4:D:54:TYR:HA	4:D:57:ARG:HB2	1.94	0.48
6:F:15:ASP:O	6:F:17:SER:N	2.46	0.48
1:A:735:C:H5'	18:R:71:LYS:HD3	1.95	0.48
1:A:1074:G:H1'	2:B:104:ASN:ND2	2.27	0.48
3:C:125:GLU:HA	3:C:191:THR:HG23	1.94	0.48
1:A:722:A:C6	1:A:724:G:C5	3.01	0.48
4:D:190:ASP:CB	4:D:192:GLU:HB3	2.43	0.48
1:A:565:U:H6	1:A:566:G:H2'	1.78	0.48
3:C:8:ILE:C	3:C:10:PHE:H	2.17	0.48
4:D:150:GLU:O	4:D:153:ARG:HB2	2.13	0.48
1:A:119:A:H4'	1:A:120:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:C:H4'	16:P:28:ARG:NH2	2.29	0.48
4:D:23:GLY:HA3	4:D:113:SER:HB3	1.95	0.48
2:B:220:ASP:C	2:B:222:ILE:H	2.17	0.48
1:A:1237:C:OP1	1:A:1238:A:H1'	2.13	0.48
1:A:797:C:H6	1:A:797:C:O5'	1.97	0.48
1:A:75:G:C6	1:A:76:C:C4	3.02	0.48
20:T:22:ARG:O	20:T:26:ASN:N	2.43	0.48
1:A:37:U:O5'	1:A:37:U:H6	1.96	0.48
1:A:939:G:H2'	1:A:940:C:H6	1.78	0.48
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.27	0.48
6:F:23:LYS:HA	6:F:26:ILE:HD12	1.94	0.48
1:A:1117:G:H5"	9:I:104:ARG:NH2	2.27	0.48
1:A:838:G:N1	1:A:840:C:H1'	2.28	0.48
1:A:677:U:H3	1:A:714:G:N2	2.03	0.48
8:H:73:ASP:OD2	8:H:75:ARG:HB2	2.13	0.48
1:A:764:C:C2	1:A:765:G:C8	3.01	0.48
1:A:1191:A:OP2	3:C:3:ASN:ND2	2.45	0.48
4:D:103:ASN:HD21	4:D:107:ARG:HG3	1.78	0.48
1:A:1092:A:C6	1:A:1183:A:C2	3.01	0.48
1:A:363:A:OP1	12:L:33:ARG:HD3	2.13	0.48
4:D:110:PHE:H	4:D:110:PHE:HD1	1.57	0.48
1:A:1487:G:H2'	1:A:1488:G:H8	1.79	0.48
1:A:1461:G:H2'	1:A:1462:G:H8	1.78	0.48
1:A:1175:G:H2'	1:A:1176:A:H8	1.77	0.48
1:A:186:C:H5'	20:T:78:ALA:HB1	1.96	0.48
4:D:208:SER:OG	4:D:209:ARG:N	2.44	0.48
1:A:63:C:N4	1:A:104:G:H1	2.12	0.48
2:B:54:THR:O	2:B:54:THR:HG22	2.14	0.48
20:T:70:SER:OG	20:T:70:SER:O	2.25	0.48
1:A:409:G:H1	1:A:433:C:H42	1.61	0.48
17:Q:87:LYS:HA	17:Q:90:ILE:HD12	1.96	0.48
3:C:173:VAL:N	3:C:174:PRO:HD3	2.29	0.48
1:A:1237:C:C5	1:A:1336:C:C4	3.02	0.48
1:A:293:G:O2'	1:A:294:U:H5'	2.14	0.48
20:T:60:GLU:O	20:T:63:ILE:HB	2.14	0.48
9:I:48:GLU:N	9:I:49:PRO:HD2	2.29	0.48
4:D:188:LEU:HB3	4:D:189:PRO:HD2	1.95	0.48
16:P:6:LEU:HB3	16:P:17:TYR:CD2	2.38	0.48
4:D:9:CYS:HB3	4:D:32:ALA:HB2	1.96	0.48
1:A:1108:G:C5	1:A:1109:C:C5	3.02	0.48
1:A:196:A:O2'	1:A:221:C:O2'	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1233:G:H2'	1:A:1234:C:C6	2.49	0.48
1:A:946:A:C2	1:A:1236:A:C2	3.01	0.48
1:A:235:C:H5'	17:Q:70:ARG:HG3	1.95	0.48
1:A:371:G:H1'	1:A:482:A:H1'	1.95	0.48
1:A:619:U:N3	4:D:134:ASP:OD2	2.47	0.48
1:A:977:A:OP1	14:N:31:ARG:NH1	2.45	0.48
1:A:562:C:C4	1:A:884:U:H5	2.30	0.48
1:A:397:A:C6	1:A:548:G:N7	2.82	0.48
7:G:70:LYS:HG2	7:G:96:GLN:HB3	1.95	0.48
1:A:1253:G:H1	1:A:1284:C:H42	1.62	0.48
13:M:67:GLU:HB3	13:M:68:GLY:H	1.51	0.48
1:A:1305:G:OP2	21:V:2:GLY:HA3	2.13	0.48
1:A:583:A:H5'	17:Q:90:ILE:HG21	1.95	0.48
1:A:1391:U:H2'	1:A:1392:G:H8	1.79	0.48
1:A:581:G:C6	1:A:758:G:C8	3.02	0.48
1:A:1159:U:C2	1:A:1182:G:C2	3.02	0.48
5:E:51:VAL:O	5:E:55:VAL:HG23	2.14	0.48
1:A:933:G:O6	7:G:3:ARG:NH2	2.47	0.48
2:B:207:ALA:HB3	2:B:210:SER:HB3	1.95	0.48
1:A:1465:C:H2'	1:A:1466:C:O4'	2.14	0.48
1:A:835:U:OP2	18:R:60:ALA:HB3	2.13	0.48
1:A:1424:C:H2'	1:A:1425:U:C6	2.49	0.48
12:L:55:VAL:HG12	12:L:68:ALA:O	2.14	0.48
2:B:62:ALA:HB1	2:B:226:ARG:HG3	1.95	0.48
5:E:89:ILE:HG12	5:E:135:THR:HG23	1.95	0.47
18:R:53:ARG:HH11	18:R:53:ARG:CG	2.27	0.47
4:D:116:GLN:O	4:D:119:GLN:N	2.45	0.47
3:C:28:GLN:O	3:C:32:LEU:HB2	2.14	0.47
1:A:581:G:H8	1:A:581:G:O5'	1.96	0.47
8:H:97:VAL:HA	8:H:100:ILE:HG13	1.96	0.47
6:F:74:ASP:HA	6:F:77:ARG:HB3	1.95	0.47
16:P:69:THR:O	16:P:72:ARG:HG2	2.13	0.47
3:C:91:LEU:O	3:C:95:THR:OG1	2.29	0.47
1:A:143:A:H2	1:A:220:G:H22	1.63	0.47
1:A:1240:U:OP2	7:G:116:ALA:N	2.47	0.47
1:A:1318:A:O2'	19:S:37:ARG:HB2	2.14	0.47
7:G:95:ARG:O	7:G:99:LEU:HD12	2.14	0.47
4:D:21:LEU:HA	4:D:21:LEU:HD23	1.57	0.47
2:B:114:ARG:HH21	2:B:118:LEU:HD11	1.79	0.47
1:A:337:C:H2'	1:A:338:A:H8	1.80	0.47
4:D:18:LYS:HB3	4:D:20:TYR:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:G:H2'	1:A:1058:G:C8	2.49	0.47
6:F:62:TRP:HB2	18:R:35:ARG:HH12	1.78	0.47
1:A:292:G:H1	1:A:308:C:N4	2.11	0.47
1:A:538:G:O3'	12:L:114:LYS:HD3	2.14	0.47
15:O:56:LEU:O	15:O:60:VAL:HG23	2.13	0.47
1:A:179:A:H2'	1:A:180:U:H6	1.78	0.47
4:D:119:GLN:HG3	4:D:123:HIS:ND1	2.29	0.47
9:I:105:ASP:C	9:I:107:ARG:H	2.17	0.47
3:C:20:SER:HB3	3:C:22:TRP:HE1	1.79	0.47
1:A:1191:A:H2'	1:A:1192:C:H6	1.79	0.47
10:J:61:GLU:HG3	10:J:62:HIS:H	1.78	0.47
1:A:976:G:O5'	1:A:1358:U:O2'	2.33	0.47
19:S:20:LEU:HA	19:S:23:ASN:HB2	1.96	0.47
1:A:1236:A:O2'	1:A:1304:G:H4'	2.14	0.47
1:A:543:C:P	4:D:14:ARG:HH11	2.37	0.47
1:A:1092:A:C6	1:A:1093:A:C6	3.02	0.47
14:N:10:ALA:HB2	14:N:21:TYR:CZ	2.49	0.47
1:A:1290:G:O2'	9:I:40:LEU:HD21	2.14	0.47
1:A:577:G:O2'	1:A:816:A:H2'	2.14	0.47
4:D:94:LEU:O	4:D:96:LEU:N	2.48	0.47
2:B:115:LEU:HG	2:B:116:GLU:N	2.28	0.47
3:C:150:LYS:HE2	3:C:167:TRP:CZ3	2.47	0.47
1:A:932:C:H4'	7:G:4:ARG:HH21	1.79	0.47
1:A:327:A:C4	1:A:329:A:C8	3.02	0.47
10:J:81:THR:O	10:J:83:GLU:N	2.48	0.47
1:A:219:C:H2'	1:A:220:G:O4'	2.15	0.47
1:A:1319:A:C8	1:A:1323:G:C6	3.03	0.47
16:P:58:TYR:O	16:P:61:SER:OG	2.24	0.47
2:B:53:ARG:HH11	2:B:53:ARG:HG3	1.79	0.47
1:A:352:C:O2'	1:A:354:G:OP1	2.28	0.47
1:A:739:C:P	6:F:2:ARG:HH22	2.38	0.47
4:D:28:SER:HB2	4:D:30:LYS:H	1.80	0.47
1:A:674:G:H2'	1:A:675:A:C8	2.40	0.47
1:A:518:C:H5"	1:A:519:C:C6	2.50	0.47
1:A:517:G:H5'	1:A:519:C:C2	2.50	0.47
1:A:1060:C:O2'	1:A:1061:G:H5'	2.15	0.47
1:A:878:G:C4	1:A:879:C:C5	3.02	0.47
1:A:390:C:O2'	16:P:28:ARG:NH2	2.48	0.47
1:A:7:G:C6	1:A:298:A:C2	3.03	0.47
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.97	0.47
12:L:46:LYS:HZ2	12:L:94:PRO:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:VAL:HG23	2:B:163:PHE:O	2.15	0.47
5:E:71:LEU:HD23	5:E:71:LEU:HA	1.71	0.47
6:F:45:LEU:HA	6:F:59:TYR:HA	1.95	0.47
9:I:16:ARG:HG3	9:I:64:THR:HB	1.96	0.47
19:S:39:THR:HG22	19:S:68:GLY:O	2.14	0.47
1:A:293:G:C6	1:A:294:U:C4	3.03	0.47
1:A:657:G:O5'	1:A:657:G:H8	1.98	0.47
1:A:1260:C:OP1	1:A:1284:C:H4'	2.15	0.47
2:B:53:ARG:NH1	2:B:53:ARG:HG3	2.29	0.47
1:A:35:G:N2	1:A:550:G:N3	2.62	0.47
1:A:487:A:H2'	1:A:488:C:O4'	2.15	0.47
1:A:340:U:H2'	1:A:341:C:C6	2.49	0.47
1:A:914:A:H2'	1:A:915:A:H5'	1.96	0.47
13:M:51:ALA:O	13:M:55:ARG:HG3	2.15	0.47
6:F:91:VAL:HG12	6:F:92:LYS:O	2.14	0.47
1:A:1326:C:H2'	1:A:1327:C:C6	2.49	0.47
7:G:15:ASP:HB3	7:G:19:GLY:H	1.80	0.47
20:T:60:GLU:HA	20:T:63:ILE:HG12	1.95	0.47
1:A:1379:G:N1	1:A:1380:U:O4	2.48	0.47
1:A:496:A:H4'	1:A:497:A:C5'	2.44	0.47
1:A:127:G:O3'	17:Q:2:PRO:HD2	2.15	0.47
14:N:14:PRO:HG2	14:N:16:PHE:O	2.15	0.47
1:A:1264:C:O2	1:A:1272:G:N2	2.48	0.47
10:J:12:ASP:HB3	10:J:14:LYS:H	1.80	0.47
8:H:69:ARG:HH21	8:H:69:ARG:HB3	1.79	0.47
3:C:94:LEU:HA	3:C:94:LEU:HD12	1.73	0.47
1:A:868:C:H2'	1:A:869:G:O4'	2.15	0.47
1:A:523:A:N6	12:L:92:ASP:HB2	2.30	0.47
4:D:186:LEU:HB3	4:D:187:ARG:HG3	1.96	0.47
1:A:1227:A:P	13:M:111:LYS:HZ3	2.37	0.47
1:A:289:G:H2'	1:A:290:C:H6	1.78	0.47
1:A:1511:G:H2'	1:A:1512:U:H6	1.80	0.47
1:A:1512:U:C2	1:A:1513:A:C8	3.03	0.47
1:A:445:G:O6	1:A:489:C:N4	2.47	0.47
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.49	0.47
1:A:503:C:H2'	1:A:504:C:H6	1.80	0.47
9:I:110:GLU:HG2	9:I:111:ARG:N	2.29	0.47
11:K:95:ILE:HG21	18:R:87:ARG:HH22	1.80	0.47
11:K:31:THR:HA	11:K:42:TRP:HA	1.96	0.47
1:A:885:G:N3	1:A:914:A:C2	2.83	0.47
1:A:582:U:N3	1:A:760:G:O6	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:C:H2'	1:A:1192:C:O2	2.15	0.46
1:A:1092:A:C6	1:A:1183:A:H2	2.33	0.46
2:B:82:ARG:O	2:B:84:GLU:N	2.49	0.46
1:A:883:C:H2'	1:A:884:U:H5'	1.97	0.46
1:A:546:G:OP1	4:D:73:ARG:HB2	2.14	0.46
15:O:42:HIS:O	15:O:46:HIS:HB2	2.15	0.46
14:N:8:GLU:OE1	14:N:11:LYS:HD2	2.15	0.46
2:B:160:ASP:O	2:B:183:PRO:HD2	2.16	0.46
1:A:1321:C:C4	1:A:1322:C:C4	3.03	0.46
1:A:544:G:H2'	1:A:545:C:O4'	2.15	0.46
17:Q:59:ILE:HG22	17:Q:72:ARG:O	2.15	0.46
1:A:1092:A:N6	1:A:1093:A:C6	2.83	0.46
1:A:688:G:H2'	1:A:689:C:C6	2.50	0.46
8:H:38:ILE:HG22	8:H:39:LEU:N	2.29	0.46
1:A:976:G:H8	1:A:1358:U:H2'	1.79	0.46
6:F:10:LEU:HD11	6:F:61:LEU:HD11	1.98	0.46
7:G:90:GLU:HG2	7:G:91:VAL:N	2.30	0.46
20:T:80:ARG:HA	20:T:83:ARG:HG3	1.97	0.46
17:Q:45:HIS:NE2	17:Q:47:PRO:HG3	2.30	0.46
1:A:1248:A:N3	9:I:70:LYS:HE3	2.30	0.46
18:R:51:LEU:HB2	18:R:56:THR:HG22	1.96	0.46
4:D:59:ARG:NH2	4:D:62:GLN:HG3	2.30	0.46
8:H:73:ASP:O	8:H:75:ARG:N	2.44	0.46
20:T:43:LEU:HA	20:T:43:LEU:HD23	1.65	0.46
1:A:445:G:H2'	1:A:446:G:C8	2.49	0.46
1:A:512:U:H2'	1:A:513:C:H6	1.78	0.46
7:G:20:ASP:HB3	7:G:23:VAL:HG23	1.97	0.46
1:A:1381:U:H2'	1:A:1381:U:O2	2.14	0.46
1:A:821:G:C2	1:A:880:C:C2	3.03	0.46
1:A:1507:A:H2'	1:A:1508:G:C8	2.51	0.46
8:H:93:VAL:CG1	8:H:133:LEU:HB3	2.41	0.46
1:A:1124:G:H4'	10:J:38:ILE:HD11	1.97	0.46
16:P:32:TYR:H	16:P:32:TYR:HD1	1.62	0.46
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.98	0.46
10:J:21:GLN:NE2	10:J:37:PRO:HG3	2.30	0.46
19:S:53:ASN:O	19:S:55:LYS:N	2.47	0.46
1:A:564:C:N3	1:A:565:U:N3	2.63	0.46
8:H:104:ARG:NH1	8:H:104:ARG:HG3	2.30	0.46
1:A:35:G:C2	1:A:550:G:C2	3.03	0.46
6:F:3:ARG:O	6:F:3:ARG:HD2	2.15	0.46
1:A:709:G:H2'	1:A:710:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:65:ASN:HA	19:S:67:VAL:HG23	1.97	0.46
1:A:192:U:H5"	20:T:57:ARG:NH2	2.31	0.46
6:F:80:ARG:NE	6:F:88:VAL:HG23	2.30	0.46
1:A:1348:U:C4	1:A:1349:A:N7	2.84	0.46
1:A:880:C:P	12:L:12:ARG:HH21	2.36	0.46
1:A:1394:A:N6	1:A:1500:A:HO2'	2.14	0.46
1:A:1394:A:N6	1:A:1501:C:H5'	2.30	0.46
1:A:578:C:O2	1:A:579:G:C8	2.69	0.46
9:I:118:LYS:HG3	9:I:121:ARG:HB3	1.98	0.46
12:L:32:PHE:O	12:L:33:ARG:HG2	2.15	0.46
16:P:51:VAL:O	16:P:52:ASP:HB3	2.15	0.46
3:C:66:VAL:O	3:C:101:LEU:HA	2.14	0.46
15:O:6:GLU:O	15:O:10:LYS:HG3	2.16	0.46
1:A:852:G:C6	1:A:853:G:N7	2.83	0.46
1:A:666:G:H5"	1:A:667:G:OP2	2.16	0.46
1:A:1485:U:H2'	1:A:1486:G:C8	2.50	0.46
1:A:1506:U:N3	1:A:1522:U:OP1	2.37	0.46
1:A:850:U:O2	1:A:851:G:C8	2.68	0.46
1:A:196:A:N3	1:A:222:U:H1'	2.30	0.46
1:A:403:C:H4'	4:D:122:ARG:CZ	2.45	0.46
1:A:499:A:H4'	1:A:500:G:H5'	1.97	0.46
1:A:277:C:OP1	17:Q:41:LYS:HE2	2.15	0.46
1:A:1461:G:H2'	1:A:1462:G:C8	2.51	0.46
2:B:90:MET:SD	2:B:91:PRO:HD2	2.55	0.46
1:A:279:A:H4'	1:A:280:C:H5"	1.97	0.46
11:K:69:ALA:O	11:K:73:MET:HG2	2.16	0.46
18:R:69:THR:HG22	18:R:70:ILE:HG13	1.97	0.46
6:F:67:MET:SD	6:F:72:VAL:HG22	2.56	0.46
3:C:24:ALA:HB3	3:C:29:TYR:CD1	2.50	0.46
17:Q:6:LEU:HB2	17:Q:59:ILE:HG13	1.98	0.46
1:A:1262:C:H2'	1:A:1263:C:C6	2.51	0.46
4:D:106:TYR:HE1	4:D:113:SER:HA	1.80	0.46
1:A:1223:C:H5"	1:A:1224:G:H5"	1.97	0.46
8:H:122:ARG:O	8:H:126:LYS:HB3	2.15	0.46
10:J:61:GLU:HG3	10:J:62:HIS:N	2.30	0.46
1:A:993:G:H4'	1:A:994:A:OP2	2.16	0.46
7:G:31:MET:SD	7:G:36:LYS:HB2	2.56	0.46
3:C:87:LEU:O	3:C:90:GLU:N	2.48	0.46
6:F:45:LEU:HB3	6:F:59:TYR:HD1	1.81	0.46
2:B:144:ARG:HB2	2:B:144:ARG:HE	1.21	0.46
3:C:138:VAL:HG13	3:C:149:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:THR:CG2	2:B:192:SER:HA	2.45	0.46
1:A:948:C:H42	1:A:1233:G:H1	1.61	0.46
18:R:69:THR:HG22	18:R:70:ILE:N	2.31	0.46
1:A:591:U:H2'	1:A:592:G:C8	2.40	0.46
4:D:135:LEU:O	4:D:138:TYR:HB2	2.16	0.46
10:J:19:SER:O	10:J:23:ILE:HG13	2.16	0.46
2:B:5:ILE:HG13	2:B:9:GLU:OE1	2.16	0.46
1:A:74:C:H2'	1:A:75:G:O4'	2.15	0.46
1:A:37:U:C2	1:A:38:G:C8	3.04	0.46
1:A:1233:G:H2'	1:A:1234:C:H6	1.80	0.46
7:G:146:GLU:C	7:G:148:ASN:H	2.18	0.46
1:A:1089:G:C5	1:A:1090:U:C5	3.03	0.46
3:C:11:ARG:O	3:C:13:GLY:N	2.48	0.46
2:B:8:LYS:HB2	2:B:8:LYS:HE3	1.84	0.46
1:A:663:A:C2	1:A:664:G:C5	3.03	0.46
1:A:889:A:C8	1:A:891:U:C2	3.04	0.46
1:A:965:A:C2	1:A:969:A:C6	3.04	0.46
4:D:128:VAL:HG22	4:D:146:ILE:CD1	2.46	0.46
1:A:540:G:H2'	1:A:541:G:O4'	2.16	0.46
1:A:1323:G:H2'	1:A:1324:A:C8	2.50	0.46
1:A:1381:U:C4	7:G:156:TRP:HH2	2.34	0.46
1:A:1291:G:H2'	1:A:1292:U:C6	2.50	0.46
1:A:79:G:C2	1:A:80:G:N7	2.84	0.46
1:A:1098:C:C2	1:A:1099:G:C8	3.03	0.46
5:E:127:ASN:HA	5:E:128:PRO:HD3	1.85	0.46
1:A:1347:G:N2	1:A:1373:G:H2'	2.31	0.46
1:A:1193:G:O2'	1:A:1194:U:H5'	2.16	0.46
1:A:1342:C:O2'	1:A:1343:G:H5'	2.15	0.46
1:A:449:C:H2'	1:A:450:G:O4'	2.16	0.46
1:A:482:A:N1	1:A:483:C:C2	2.84	0.46
2:B:149:LEU:C	2:B:151:GLY:H	2.19	0.46
4:D:26:CYS:HA	4:D:31:CYS:HB3	1.97	0.46
19:S:44:MET:HA	19:S:47:HIS:CD2	2.49	0.46
18:R:23:LYS:HD2	18:R:57:GLY:O	2.16	0.46
16:P:81:ARG:HG3	16:P:82:GLN:N	2.30	0.46
13:M:80:ARG:O	13:M:84:ILE:HG13	2.15	0.46
1:A:175:C:H4'	20:T:25:ARG:NH1	2.31	0.46
17:Q:29:HIS:HA	17:Q:30:PRO:HD2	1.73	0.45
1:A:820:U:H4'	1:A:821:G:OP2	2.15	0.45
1:A:571:U:H5"	1:A:572:A:OP2	2.16	0.45
13:M:10:PRO:CB	13:M:13:LYS:HD3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1518:A:C4	1:A:1519:A:N7	2.83	0.45
6:F:11:ASN:HD22	6:F:13:ASN:ND2	2.14	0.45
11:K:64:ALA:C	11:K:66:LEU:H	2.20	0.45
1:A:99:C:H2'	1:A:101:A:C8	2.51	0.45
2:B:33:TYR:HB2	2:B:41:ILE:HG22	1.98	0.45
1:A:1179:A:H4'	9:I:103:THR:HA	1.98	0.45
1:A:1077:G:N2	1:A:1080:A:OP2	2.39	0.45
18:R:53:ARG:HD2	18:R:63:GLN:HB3	1.97	0.45
1:A:946:A:O2'	1:A:1333:A:N3	2.27	0.45
3:C:23:TYR:CG	3:C:24:ALA:N	2.84	0.45
1:A:542:G:H2'	1:A:543:C:H6	1.81	0.45
1:A:577:G:H1'	1:A:816:A:N3	2.31	0.45
1:A:482:A:N3	1:A:482:A:H2'	2.31	0.45
4:D:94:LEU:HD23	4:D:94:LEU:HA	1.65	0.45
1:A:688:G:H2'	1:A:689:C:H6	1.81	0.45
1:A:329:A:C2	1:A:332:G:C4	3.04	0.45
1:A:1518:A:H8	1:A:1518:A:OP2	2.00	0.45
1:A:656:C:H4'	15:O:62:GLN:OE1	2.16	0.45
1:A:1039:C:H2'	1:A:1040:U:H6	1.81	0.45
3:C:134:ILE:CG2	3:C:151:VAL:HB	2.46	0.45
3:C:164:ARG:HB2	3:C:165:THR:H	1.49	0.45
6:F:50:TYR:N	6:F:50:TYR:CD2	2.84	0.45
1:A:430:A:OP2	4:D:22:LYS:HE2	2.17	0.45
1:A:390:C:O3'	16:P:28:ARG:NH2	2.40	0.45
5:E:37:ARG:O	5:E:114:GLY:HA3	2.16	0.45
5:E:144:THR:C	5:E:146:ALA:H	2.18	0.45
1:A:50:A:N6	1:A:361:G:H4'	2.31	0.45
8:H:80:ILE:H	8:H:80:ILE:HG12	1.49	0.45
14:N:40:CYS:SG	14:N:42:ILE:N	2.89	0.45
1:A:951:G:N3	1:A:970:C:O2'	2.38	0.45
1:A:331:G:OP1	1:A:332:G:H8	2.00	0.45
6:F:63:TYR:O	6:F:65:VAL:HG13	2.16	0.45
1:A:1001:A:C6	1:A:1002:G:C6	3.04	0.45
1:A:226:G:H2'	1:A:227:G:H8	1.80	0.45
1:A:500:G:C6	1:A:546:G:C2	3.04	0.45
1:A:302:G:N3	1:A:556:C:H4'	2.32	0.45
4:D:21:LEU:HD21	4:D:114:ARG:HB2	1.98	0.45
1:A:43:C:H2'	1:A:44:G:O4'	2.16	0.45
20:T:49:ALA:O	20:T:53:LEU:HG	2.16	0.45
1:A:1073:U:H2'	1:A:1074:G:O4'	2.17	0.45
1:A:760:G:N2	17:Q:94:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:A:H3'	1:A:1503:A:C5'	2.46	0.45
1:A:1151:A:O2'	1:A:1152:A:H8	1.99	0.45
1:A:577:G:C2	1:A:578:C:C6	3.04	0.45
1:A:1314:C:C2	1:A:1315:U:C5	3.04	0.45
1:A:655:A:H61	1:A:752:G:N2	2.15	0.45
1:A:1435:G:O5'	1:A:1435:G:H8	1.99	0.45
11:K:33:THR:HG22	11:K:39:PRO:HA	1.98	0.45
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.15	0.45
2:B:73:THR:HG23	2:B:95:GLN:O	2.17	0.45
8:H:59:LEU:HA	8:H:59:LEU:HD23	1.83	0.45
1:A:316:G:H5"	1:A:353:A:N6	2.32	0.45
1:A:1062:U:H2'	1:A:1063:C:C6	2.52	0.45
1:A:195:A:N7	1:A:196:A:N6	2.65	0.45
7:G:105:VAL:O	7:G:107:ALA:N	2.50	0.45
1:A:925:G:C2	1:A:927:G:C8	3.05	0.45
18:R:60:ALA:O	18:R:64:ARG:NH1	2.49	0.45
3:C:44:GLU:O	3:C:46:GLU:N	2.50	0.45
1:A:694:A:N1	1:A:787:A:O2'	2.50	0.45
1:A:1364:U:O2'	1:A:1365:G:H5'	2.16	0.45
1:A:857:C:N4	1:A:858:G:C6	2.84	0.45
1:A:515:G:C2	1:A:537:G:C2	3.05	0.45
3:C:24:ALA:HB3	3:C:29:TYR:HD1	1.81	0.45
1:A:651:C:H2'	1:A:652:U:C5	2.50	0.45
3:C:172:ARG:HH21	3:C:174:PRO:HG3	1.81	0.45
20:T:43:LEU:HD13	20:T:51:GLU:HB2	1.98	0.45
12:L:42:THR:HG22	12:L:54:LYS:HA	1.99	0.45
1:A:643:C:H5'	8:H:31:PHE:CZ	2.52	0.45
1:A:44:G:OP2	16:P:12:LYS:HB2	2.16	0.45
1:A:1309:G:C6	1:A:1329:A:C2	3.04	0.45
1:A:463:A:P	16:P:75:ARG:HH12	2.39	0.45
1:A:1278:U:H5"	1:A:1279:A:H5'	1.99	0.45
1:A:173:U:H5	1:A:198:G:HO2'	1.65	0.45
1:A:1136:U:OP2	1:A:1137:C:N4	2.50	0.45
13:M:90:LEU:HA	13:M:93:ARG:NH1	2.31	0.45
1:A:777:A:H2	11:K:119:CYS:HG	1.63	0.45
1:A:575:G:C4	1:A:881:G:N2	2.85	0.45
18:R:72:ARG:C	18:R:74:ARG:H	2.19	0.45
2:B:54:THR:O	2:B:55:PHE:HD1	1.99	0.45
2:B:47:THR:OG1	2:B:202:PRO:HG2	2.17	0.45
1:A:499:A:H4'	1:A:500:G:OP1	2.16	0.45
4:D:65:ARG:HE	4:D:72:GLU:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:188:LEU:HD11	3:C:195:VAL:HG22	1.99	0.45
3:C:178:LEU:O	3:C:180:ALA:N	2.50	0.45
2:B:37:ASN:O	2:B:39:ILE:N	2.50	0.45
1:A:190(F):G:OP1	1:A:190(F):G:H8	2.00	0.45
1:A:719:C:H3'	1:A:720:C:H5	1.82	0.45
3:C:32:LEU:HD13	3:C:59:ARG:HE	1.81	0.45
4:D:43:HIS:HB3	4:D:46:LYS:HD2	1.99	0.45
4:D:103:ASN:ND2	4:D:107:ARG:HG3	2.31	0.45
14:N:37:PHE:HB3	14:N:39:LEU:HB2	1.99	0.45
12:L:69:TYR:HD2	12:L:99:HIS:CD2	2.35	0.45
5:E:11:ILE:HG21	5:E:31:LEU:HD23	1.98	0.45
1:A:279:A:H5"	1:A:280:C:H3'	1.99	0.45
1:A:767:A:H2'	1:A:768:A:C8	2.52	0.45
1:A:1081:G:H2'	1:A:1082:G:C8	2.52	0.45
1:A:1107:C:N4	1:A:1108:G:N7	2.65	0.45
1:A:939:G:H2'	1:A:940:C:C6	2.52	0.45
2:B:115:LEU:O	2:B:119:GLU:HG3	2.16	0.45
5:E:111:GLU:O	5:E:114:GLY:N	2.48	0.45
4:D:104:VAL:CG1	4:D:146:ILE:HG13	2.46	0.45
1:A:1184:G:O2'	1:A:1185:G:H5'	2.16	0.45
1:A:771:G:C2	1:A:809:G:C2	3.05	0.45
1:A:975:A:H5'	1:A:975:A:H8	1.80	0.45
1:A:707:C:H4'	11:K:20:TYR:CD1	2.52	0.45
11:K:34:ASP:O	11:K:37:GLY:N	2.49	0.45
1:A:598:U:O2'	8:H:94:TYR:HB3	2.17	0.45
1:A:985:C:H2'	1:A:986:A:H8	1.81	0.45
15:O:27:VAL:HG12	15:O:31:LEU:HD11	1.99	0.45
1:A:616:G:H1'	1:A:625:G:N2	2.32	0.45
15:O:8:LYS:O	15:O:9:GLN:C	2.54	0.45
2:B:62:ALA:O	2:B:226:ARG:HG2	2.17	0.45
18:R:43:PHE:O	18:R:44:LEU:HD23	2.17	0.45
1:A:352:C:O2'	1:A:353:A:H5"	2.17	0.45
1:A:1521:G:H2'	1:A:1522:U:O4'	2.17	0.45
1:A:577:G:C4	1:A:816:A:C2	3.05	0.45
2:B:105:PHE:O	2:B:109:SER:HB2	2.16	0.45
1:A:571:U:C3'	1:A:572:A:H5"	2.45	0.45
5:E:93:PRO:HG2	8:H:105:ARG:CZ	2.47	0.45
1:A:922:G:C2	1:A:1396:A:C2	3.05	0.45
1:A:560:U:H5"	1:A:561:U:H5"	1.99	0.45
8:H:7:ALA:HB2	8:H:85:ARG:HD3	1.98	0.45
1:A:475:G:H2'	1:A:476:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:C:H1'	1:A:1468:A:H2	1.82	0.45
1:A:1319:A:C8	1:A:1323:G:C5	3.05	0.45
6:F:3:ARG:O	6:F:93:SER:HB2	2.17	0.45
3:C:93:LYS:HE3	3:C:93:LYS:HB2	1.80	0.45
3:C:89:GLU:O	3:C:93:LYS:N	2.46	0.45
1:A:876:G:C6	1:A:877:C:N4	2.85	0.45
1:A:978:A:H1'	1:A:1322:C:O2	2.17	0.44
1:A:1119:C:H2'	1:A:1120:G:H8	1.79	0.44
8:H:16:ALA:O	8:H:19:VAL:HB	2.16	0.44
1:A:730:G:C2	1:A:765:G:H4'	2.52	0.44
1:A:1366:C:H2'	1:A:1367:C:C6	2.42	0.44
4:D:51:PRO:HB2	4:D:56:VAL:HG23	1.99	0.44
20:T:13:LEU:HG	20:T:13:LEU:H	1.46	0.44
1:A:20:U:H2'	1:A:21:G:O4'	2.18	0.44
5:E:41:VAL:HB	5:E:113:ALA:HA	1.99	0.44
11:K:22:HIS:HB3	11:K:29:ILE:HB	1.99	0.44
4:D:25:ARG:HH21	4:D:30:LYS:HB3	1.82	0.44
15:O:30:ALA:O	15:O:33:THR:N	2.50	0.44
4:D:23:GLY:H	4:D:26:CYS:HB2	1.82	0.44
5:E:99:GLY:H	5:E:117:ASP:HB3	1.81	0.44
1:A:627:G:H2'	1:A:628:G:C8	2.52	0.44
1:A:754:C:H2'	1:A:754:C:O2	2.17	0.44
20:T:10:LEU:HD23	20:T:13:LEU:HD12	1.99	0.44
1:A:244:U:O4'	1:A:894:G:N2	2.49	0.44
5:E:110:LEU:HD13	5:E:118:ILE:HD13	2.00	0.44
1:A:828:A:OP1	8:H:21:LYS:NZ	2.50	0.44
15:O:32:LEU:O	15:O:35:ARG:N	2.51	0.44
2:B:73:THR:OG1	2:B:170:GLU:OE2	2.30	0.44
4:D:56:VAL:HG12	4:D:202:LEU:HD11	1.98	0.44
4:D:77:ASN:O	4:D:81:GLU:HB2	2.17	0.44
8:H:56:LYS:HA	8:H:56:LYS:HD3	1.49	0.44
1:A:59:A:H4'	1:A:388:G:OP1	2.18	0.44
1:A:650:G:C2	1:A:651:C:C6	3.04	0.44
1:A:576:G:H3'	1:A:577:G:C5'	2.46	0.44
12:L:89:ARG:CG	12:L:90:VAL:H	2.29	0.44
5:E:99:GLY:CA	5:E:117:ASP:HA	2.45	0.44
1:A:613:C:O2	1:A:628:G:N2	2.50	0.44
1:A:589:C:C2	1:A:590:C:C5	3.06	0.44
1:A:116:A:H2	1:A:314:C:HO2'	1.64	0.44
1:A:983:A:H2	1:A:984:C:C6	2.35	0.44
11:K:77:MET:HG3	11:K:103:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:50:ILE:HD11	7:G:121:ALA:HA	1.99	0.44
1:A:315:A:H5"	1:A:317:G:OP2	2.17	0.44
5:E:18:ARG:O	5:E:19:MET:HG2	2.17	0.44
4:D:119:GLN:HG3	4:D:123:HIS:CE1	2.53	0.44
1:A:376:G:OP2	16:P:67:THR:HG21	2.17	0.44
1:A:1506:U:O2'	1:A:1507:A:H5'	2.16	0.44
1:A:1367:C:C2	1:A:1368:G:C8	3.06	0.44
2:B:108:ILE:O	2:B:111:ARG:N	2.45	0.44
1:A:1228:C:OP1	13:M:115:LYS:N	2.44	0.44
1:A:41:G:C2	1:A:402:G:C2	3.06	0.44
1:A:1299:A:H2'	1:A:1301:U:C6	2.53	0.44
11:K:33:THR:HG22	11:K:39:PRO:N	2.32	0.44
18:R:28:GLU:H	18:R:28:GLU:HG2	1.50	0.44
15:O:24:SER:O	15:O:28:GLN:NE2	2.51	0.44
1:A:709:G:H2'	1:A:710:G:C8	2.51	0.44
4:D:49:ARG:HD2	4:D:49:ARG:H	1.83	0.44
1:A:892:A:C2	1:A:893:C:C2	3.05	0.44
1:A:383:A:C5	1:A:384:G:H1'	2.52	0.44
4:D:11:LEU:C	4:D:13:ARG:N	2.68	0.44
1:A:1376:U:H2'	1:A:1377:A:C8	2.52	0.44
1:A:66:G:N3	1:A:66:G:H2'	2.31	0.44
14:N:42:ILE:HG22	14:N:46:GLU:OE1	2.17	0.44
1:A:807:A:H5"	1:A:808:C:OP2	2.17	0.44
1:A:1238:A:OP2	1:A:1335:C:H1'	2.18	0.44
1:A:227:G:H2'	1:A:228:A:O4'	2.18	0.44
1:A:1489:G:H2'	1:A:1490:C:C6	2.52	0.44
12:L:25:PRO:HG2	12:L:98:TYR:OH	2.18	0.44
1:A:1527:C:C2'	1:A:1528:U:H5'	2.48	0.44
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.51	0.44
17:Q:81:ARG:O	17:Q:84:LEU:HD12	2.17	0.44
8:H:29:SER:HB2	8:H:32:LYS:H	1.83	0.44
1:A:1354:C:H6	1:A:1354:C:O5'	2.01	0.44
1:A:353:A:H2'	1:A:353:A:N3	2.32	0.44
3:C:125:GLU:HG2	3:C:190:ARG:H	1.82	0.44
1:A:1305:G:C2	1:A:1331:G:N3	2.86	0.44
1:A:673:G:H5"	6:F:87:ARG:HH11	1.83	0.44
1:A:581:G:C6	1:A:758:G:N7	2.86	0.44
1:A:974:A:C8	14:N:31:ARG:HD2	2.53	0.44
1:A:970:C:H42	9:I:127:LYS:HD3	1.82	0.44
5:E:34:VAL:HG12	5:E:35:GLY:N	2.33	0.44
1:A:726:C:H2'	1:A:727:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:G:C6	1:A:491:G:C5	3.06	0.44
12:L:22:SER:O	12:L:22:SER:OG	2.35	0.44
7:G:136:LYS:O	7:G:140:ASP:HB2	2.16	0.44
8:H:113:SER:HA	8:H:117:GLY:O	2.18	0.44
1:A:373:A:C5	1:A:482:A:N7	2.86	0.44
1:A:62:U:C2	1:A:63:C:C5	3.05	0.44
4:D:101:LEU:HD23	4:D:121:VAL:HG13	1.99	0.44
1:A:1488:G:H2'	1:A:1489:G:C8	2.51	0.44
9:I:89:ASN:C	9:I:91:ASP:H	2.22	0.44
1:A:1480:G:H2'	1:A:1481:U:H6	1.83	0.44
8:H:127:LEU:HD23	8:H:127:LEU:HA	1.68	0.44
1:A:737:A:OP1	6:F:92:LYS:N	2.50	0.44
1:A:24:U:OP1	12:L:23:LYS:NZ	2.48	0.44
2:B:176:GLU:C	2:B:178:ARG:H	2.21	0.44
8:H:91:ARG:HB2	12:L:7:ILE:HG13	2.00	0.44
8:H:104:ARG:HG2	8:H:138:TRP:CE3	2.53	0.44
1:A:438:G:O2'	1:A:495:U:O4	2.35	0.44
3:C:84:ILE:CD1	3:C:88:ARG:HH22	2.31	0.44
1:A:276:G:OP1	17:Q:12:SER:OG	2.36	0.44
5:E:36:ASP:C	5:E:38:GLN:H	2.20	0.43
1:A:940:C:C2	1:A:941:G:C8	3.06	0.43
4:D:31:CYS:O	4:D:33:MET:N	2.51	0.43
1:A:973:G:OP1	10:J:57:LYS:NZ	2.26	0.43
1:A:335:C:H2'	1:A:336:C:H6	1.80	0.43
3:C:52:LEU:HD12	3:C:69:HIS:O	2.18	0.43
9:I:79:LEU:HD12	9:I:79:LEU:HA	1.91	0.43
1:A:981:U:OP1	14:N:9:LYS:HD2	2.18	0.43
1:A:344:A:H5"	1:A:345:C:C5	2.53	0.43
5:E:148:VAL:C	5:E:150:ARG:H	2.21	0.43
1:A:1497:G:C6	1:A:1498:U:N3	2.86	0.43
1:A:9:G:H5'	5:E:122:GLU:CD	2.39	0.43
6:F:2:ARG:O	6:F:4:TYR:HE2	2.01	0.43
1:A:1190:G:O2'	3:C:3:ASN:HB2	2.18	0.43
3:C:7:PRO:CG	3:C:184:TYR:HB2	2.44	0.43
4:D:18:LYS:O	4:D:19:LEU:HD23	2.17	0.43
10:J:61:GLU:OE2	14:N:58:LYS:HD3	2.18	0.43
3:C:123:GLN:HA	3:C:126:ARG:HB2	1.99	0.43
3:C:138:VAL:HG22	3:C:151:VAL:HG23	2.00	0.43
1:A:1118:C:OP1	9:I:104:ARG:NE	2.45	0.43
3:C:11:ARG:O	3:C:14:ILE:N	2.45	0.43
4:D:30:LYS:HG2	4:D:35:ARG:HH21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:C:H1'	1:A:622:A:H1'	2.00	0.43
1:A:516:U:C4	1:A:517:G:C6	3.07	0.43
1:A:1502:A:OP1	1:A:1502:A:H4'	2.16	0.43
8:H:89:PRO:HB3	8:H:92:ARG:NH2	2.33	0.43
5:E:107:ARG:O	5:E:111:GLU:HB2	2.18	0.43
12:L:46:LYS:NZ	12:L:94:PRO:HG3	2.33	0.43
4:D:106:TYR:CE1	4:D:113:SER:HA	2.52	0.43
1:A:972:C:H4'	10:J:57:LYS:HD2	2.00	0.43
11:K:20:TYR:HB2	11:K:31:THR:O	2.17	0.43
15:O:18:PHE:HD2	15:O:21:ASP:HB2	1.83	0.43
9:I:26:VAL:HA	9:I:61:ALA:HB3	2.00	0.43
21:V:13:ILE:HG12	21:V:22:ARG:HD2	2.00	0.43
8:H:88:LYS:HB2	8:H:88:LYS:HE3	1.88	0.43
17:Q:94:ASN:O	17:Q:97:SER:OG	2.28	0.43
6:F:76:ALA:HA	6:F:79:LEU:HG	2.00	0.43
8:H:20:TYR:CE2	8:H:75:ARG:HG2	2.53	0.43
1:A:11:G:H1	1:A:23:C:N4	2.15	0.43
4:D:101:LEU:HD12	4:D:101:LEU:HA	1.79	0.43
1:A:973:G:O5'	1:A:973:G:H8	2.01	0.43
8:H:37:ARG:NH1	8:H:38:ILE:HG13	2.34	0.43
8:H:38:ILE:HG21	8:H:111:ILE:CD1	2.47	0.43
15:O:53:HIS:O	15:O:56:LEU:HB3	2.18	0.43
1:A:902:G:H2'	1:A:903:G:C8	2.54	0.43
1:A:1261:A:C6	1:A:1275:A:C4	3.06	0.43
1:A:123:C:O5'	1:A:123:C:H6	2.00	0.43
14:N:15:LYS:HD3	14:N:15:LYS:HA	1.61	0.43
8:H:87:SER:HB2	8:H:133:LEU:O	2.19	0.43
3:C:150:LYS:NZ	3:C:173:VAL:HG11	2.33	0.43
1:A:771:G:H1	1:A:808:C:H42	1.66	0.43
13:M:108:ARG:NH2	13:M:111:LYS:HD2	2.32	0.43
8:H:6:ILE:HD11	8:H:31:PHE:HD2	1.80	0.43
13:M:30:ALA:O	13:M:33:ALA:N	2.44	0.43
1:A:623:C:H6	1:A:623:C:O5'	2.01	0.43
1:A:132:C:H2'	1:A:133:U:O4'	2.19	0.43
1:A:431:A:N3	1:A:431:A:H2'	2.33	0.43
1:A:1507:A:C2	1:A:1508:G:C5	3.06	0.43
1:A:964:A:H5"	1:A:965:A:OP2	2.18	0.43
1:A:1104:G:H4'	2:B:111:ARG:HH11	1.84	0.43
1:A:923:A:H2	1:A:1395:C:O2	2.00	0.43
1:A:437:U:H5"	4:D:155:LEU:HD11	2.00	0.43
1:A:701:C:H1'	1:A:703:G:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:G:OP2	13:M:102:ARG:NH2	2.51	0.43
1:A:1126:U:O2'	1:A:1280:A:H8	2.01	0.43
1:A:986:A:H4'	19:S:55:LYS:HD2	2.01	0.43
1:A:243:A:C2	1:A:245:C:C2	3.07	0.43
9:I:26:VAL:HB	9:I:33:PHE:HB2	2.01	0.43
1:A:452:A:C2	1:A:453:A:C4	3.07	0.43
16:P:39:TYR:CE2	16:P:41:PRO:HG3	2.52	0.43
3:C:125:GLU:HG3	3:C:189:ALA:HB1	2.00	0.43
7:G:12:LEU:HB3	7:G:24:THR:HG21	2.01	0.43
1:A:968:A:C8	1:A:1062:U:H4'	2.54	0.43
1:A:716:A:O2'	1:A:717:C:H5'	2.18	0.43
1:A:67:C:H2'	1:A:68:G:C8	2.51	0.43
15:O:24:SER:H	15:O:27:VAL:HG21	1.84	0.43
1:A:538:G:OP1	12:L:114:LYS:N	2.47	0.43
11:K:73:MET:HA	11:K:77:MET:H	1.84	0.43
1:A:637:G:C4	1:A:638:G:C8	3.07	0.43
7:G:100:ALA:O	7:G:104:LEU:HG	2.19	0.43
20:T:21:LYS:HB3	20:T:21:LYS:HE3	1.86	0.43
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.83	0.43
12:L:10:LEU:HA	12:L:14:GLY:H	1.84	0.43
2:B:105:PHE:CB	2:B:158:LEU:HD21	2.48	0.43
2:B:70:PHE:O	2:B:93:VAL:N	2.47	0.43
1:A:403:C:H4'	4:D:122:ARG:NH1	2.33	0.43
5:E:34:VAL:CG1	5:E:35:GLY:N	2.82	0.43
9:I:29:ASN:OD1	9:I:64:THR:HA	2.18	0.43
1:A:927:G:H2'	1:A:928:G:C8	2.52	0.43
1:A:538:G:H5"	12:L:114:LYS:HB2	2.01	0.43
1:A:988:G:N2	1:A:1217:C:O2	2.52	0.43
1:A:13:U:O2	1:A:914:A:H8	2.00	0.43
16:P:1:MET:CE	16:P:3:LYS:HD2	2.49	0.43
2:B:182:ILE:HG22	2:B:183:PRO:O	2.19	0.43
1:A:1206:G:C5	1:A:1207:G:C5	3.07	0.43
1:A:757:U:OP1	1:A:822:C:O2'	2.26	0.43
1:A:370:C:N3	1:A:392:G:N2	2.66	0.43
1:A:297:G:N2	1:A:299:G:O5'	2.52	0.43
4:D:18:LYS:HE3	4:D:33:MET:HB3	2.00	0.43
1:A:864:A:C2	1:A:865:A:C2	3.06	0.43
19:S:3:ARG:HD3	19:S:4:SER:N	2.33	0.43
16:P:22:THR:OG1	16:P:26:ARG:HD2	2.19	0.43
6:F:12:PRO:HB2	6:F:45:LEU:HD12	2.01	0.43
1:A:988:G:O2'	1:A:1016:A:N1	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:37:PHE:HE1	9:I:70:LYS:HB3	1.84	0.43
3:C:108:ASN:HA	3:C:109:PRO:HD3	1.72	0.43
9:I:122:ALA:HB1	9:I:123:PRO:HD2	2.00	0.43
1:A:943:U:H1'	9:I:124:GLN:OE1	2.19	0.43
19:S:71:LEU:HD23	19:S:71:LEU:HA	1.77	0.43
3:C:26:LYS:HG3	3:C:26:LYS:H	1.45	0.43
1:A:778:G:H1	1:A:804:U:H3	1.66	0.43
1:A:979:C:C2'	1:A:980:C:H5'	2.43	0.43
3:C:22:TRP:CH2	3:C:32:LEU:HB3	2.54	0.43
1:A:938:A:C6	1:A:939:G:C5	3.07	0.43
1:A:11:G:H1	1:A:23:C:H42	1.65	0.43
1:A:62:U:H5"	1:A:385:C:O2'	2.19	0.43
4:D:173:TRP:C	4:D:186:LEU:HB2	2.39	0.43
8:H:100:ILE:HD12	8:H:125:ARG:HG3	2.01	0.43
1:A:564:C:H5'	17:Q:32:TYR:HE2	1.82	0.43
12:L:6:THR:H	12:L:9:GLN:HG3	1.84	0.43
1:A:1462:G:H2'	1:A:1463:C:C6	2.54	0.43
2:B:94:ASN:OD1	2:B:95:GLN:N	2.52	0.43
7:G:78:ARG:O	7:G:84:ASN:HB2	2.19	0.43
1:A:158:G:N2	1:A:162:A:H62	2.17	0.43
1:A:682:G:H2'	1:A:683:G:C8	2.53	0.43
5:E:122:GLU:HG2	5:E:131:ILE:HG21	2.01	0.42
1:A:417:C:N4	1:A:426:G:H1	2.17	0.42
1:A:410:G:H2'	1:A:429:U:C4	2.54	0.42
1:A:327:A:C2	1:A:329:A:C4	3.07	0.42
1:A:1357:A:H5"	1:A:1358:U:OP2	2.19	0.42
6:F:40:VAL:HG22	6:F:63:TYR:HA	2.01	0.42
1:A:293:G:C5	1:A:294:U:C4	3.06	0.42
1:A:1015:A:C6	1:A:1016:A:C5	3.07	0.42
1:A:119:A:C5	1:A:240:C:C4	3.07	0.42
2:B:125:PRO:O	2:B:128:GLU:HG3	2.19	0.42
1:A:862:C:O2'	1:A:863:U:H5'	2.19	0.42
8:H:109:ILE:HA	8:H:109:ILE:HD12	1.71	0.42
1:A:1306:A:H1'	1:A:1332:A:C2	2.55	0.42
21:V:2:GLY:O	21:V:10:ARG:HG3	2.20	0.42
1:A:517:G:N2	1:A:533:A:OP2	2.52	0.42
3:C:40:ARG:HD3	3:C:55:VAL:HB	2.01	0.42
4:D:10:ARG:HG3	4:D:40:PRO:CG	2.48	0.42
5:E:110:LEU:HD22	5:E:118:ILE:HD13	2.01	0.42
1:A:523:A:C2	1:A:527:G:C6	3.07	0.42
2:B:70:PHE:CD2	2:B:163:PHE:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:G:OP1	1:A:974:A:H5"	2.18	0.42
1:A:500:G:N2	1:A:546:G:H1'	2.34	0.42
1:A:1527:C:N4	1:A:1528:U:O4	2.52	0.42
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.53	0.42
5:E:148:VAL:C	5:E:150:ARG:N	2.73	0.42
1:A:188:C:H5'	20:T:89:ARG:HD3	2.00	0.42
2:B:132:LYS:HA	2:B:135:GLN:HB2	2.01	0.42
10:J:39:PRO:HA	10:J:70:ARG:CZ	2.49	0.42
1:A:1442:G:H4'	1:A:1446:A:O4'	2.19	0.42
1:A:28:G:C2	1:A:29:G:C8	3.06	0.42
17:Q:89:LEU:HD23	17:Q:89:LEU:HA	1.76	0.42
1:A:1101:A:H4'	1:A:1102:A:C4'	2.49	0.42
1:A:720:C:H6	1:A:720:C:O5'	2.03	0.42
6:F:92:LYS:HB3	6:F:92:LYS:HE2	1.46	0.42
1:A:265:G:H5'	17:Q:64:PRO:O	2.19	0.42
7:G:9:VAL:HG11	7:G:94:ARG:HD2	2.00	0.42
1:A:577:G:C4	1:A:578:C:H5	2.37	0.42
2:B:111:ARG:HB3	2:B:111:ARG:HE	1.51	0.42
1:A:5:U:H4'	1:A:6:G:O4'	2.19	0.42
12:L:46:LYS:HA	12:L:46:LYS:HD2	1.86	0.42
8:H:78:GLN:C	8:H:80:ILE:N	2.71	0.42
1:A:933:G:N2	1:A:1384:C:O2	2.47	0.42
8:H:85:ARG:NH1	8:H:134:ILE:HG23	2.33	0.42
4:D:127:THR:HG23	4:D:130:GLY:HA2	2.01	0.42
1:A:1328:C:O3'	13:M:29:ARG:HG3	2.19	0.42
1:A:1015:A:C4	1:A:1016:A:C8	3.07	0.42
19:S:33:THR:HG22	19:S:34:TRP:H	1.84	0.42
3:C:8:ILE:O	3:C:10:PHE:N	2.53	0.42
1:A:532:A:C3'	1:A:533:A:H5'	2.50	0.42
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.34	0.42
1:A:978:A:H5'	1:A:979:C:OP2	2.20	0.42
1:A:502:G:H2'	1:A:503:C:O4'	2.20	0.42
5:E:13:ILE:HD11	5:E:55:VAL:HG22	2.01	0.42
3:C:120:VAL:HG12	3:C:124:ILE:HD11	2.02	0.42
2:B:88:ALA:HB2	2:B:219:VAL:HG13	2.01	0.42
1:A:771:G:N3	1:A:809:G:C2	2.87	0.42
6:F:12:PRO:HD3	6:F:58:GLY:HA2	2.02	0.42
10:J:40:LEU:HA	10:J:41:PRO:HD2	1.77	0.42
5:E:34:VAL:CG1	5:E:35:GLY:H	2.32	0.42
1:A:1317:C:N3	19:S:37:ARG:NH2	2.65	0.42
1:A:1220:G:H2'	1:A:1221:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:U:C6	1:A:566:G:C8	3.07	0.42
16:P:11:SER:HB2	16:P:12:LYS:H	1.73	0.42
1:A:1242:C:H6	1:A:1242:C:O5'	2.01	0.42
2:B:187:LEU:HD12	2:B:201:ILE:HB	2.01	0.42
4:D:169:LYS:HG3	4:D:170:VAL:H	1.83	0.42
1:A:824:C:H1'	8:H:1:MET:O	2.20	0.42
11:K:51:LYS:HB3	11:K:51:LYS:HE2	1.73	0.42
9:I:55:ALA:HB1	9:I:58:HIS:HB2	2.01	0.42
1:A:517:G:H4'	1:A:519:C:C5	2.55	0.42
1:A:23:C:O3'	12:L:23:LYS:NZ	2.52	0.42
12:L:93:LEU:HA	12:L:94:PRO:HD3	1.63	0.42
1:A:57:G:O6	1:A:356:A:N6	2.53	0.42
1:A:146:G:C2	1:A:147:G:C5	3.08	0.42
16:P:38:TYR:CE2	16:P:50:LYS:HB3	2.54	0.42
1:A:125:U:N3	1:A:126:G:N7	2.67	0.42
17:Q:81:ARG:HG3	17:Q:84:LEU:HD11	2.00	0.42
7:G:78:ARG:HG2	7:G:79:ARG:H	1.85	0.42
17:Q:4:LYS:O	17:Q:60:ILE:HA	2.20	0.42
1:A:1004:A:C2	1:A:1026:G:C4	3.07	0.42
5:E:121:LYS:NZ	5:E:122:GLU:O	2.52	0.42
17:Q:64:PRO:HB3	17:Q:70:ARG:NH1	2.24	0.42
1:A:380:G:C2	1:A:384:G:C6	3.07	0.42
2:B:44:LEU:O	2:B:48:MET:HG2	2.20	0.42
1:A:746:A:H4'	1:A:837:G:O2'	2.20	0.42
3:C:201:TYR:N	3:C:201:TYR:CD1	2.88	0.42
2:B:51:LEU:HD22	2:B:51:LEU:HA	1.68	0.42
6:F:22:GLU:C	6:F:24:GLU:H	2.22	0.42
1:A:976:G:N7	1:A:1358:U:C2	2.87	0.42
1:A:1280:A:N3	10:J:41:PRO:HG3	2.34	0.42
1:A:176:C:H2'	1:A:177:C:H6	1.84	0.42
1:A:1218:C:H5"	1:A:1219:U:OP2	2.19	0.42
7:G:70:LYS:HB3	7:G:96:GLN:OE1	2.20	0.42
5:E:61:TYR:HA	5:E:64:ARG:HD3	2.01	0.42
1:A:1348:U:O3'	9:I:120:ARG:HB2	2.19	0.42
1:A:517:G:N1	1:A:533:A:OP2	2.53	0.42
2:B:176:GLU:O	2:B:179:LYS:N	2.49	0.42
2:B:108:ILE:HG21	2:B:152:PHE:CE2	2.54	0.42
1:A:1226:C:H4'	1:A:1227:A:OP1	2.19	0.42
13:M:48:LEU:HD13	13:M:53:VAL:HG22	2.00	0.42
1:A:147:G:H2'	1:A:148:G:C8	2.55	0.42
6:F:3:ARG:NH1	6:F:38:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:C:N4	1:A:491:G:N1	2.68	0.42
1:A:453:A:C5	1:A:454:C:C4	3.07	0.42
3:C:50:ALA:O	3:C:71:ALA:HB3	2.20	0.42
1:A:552:U:H6	1:A:552:U:O5'	2.02	0.42
5:E:131:ILE:HA	5:E:134:ALA:CB	2.49	0.42
4:D:22:LYS:HA	4:D:22:LYS:HD3	2.00	0.42
12:L:110:VAL:O	12:L:122:THR:OG1	2.29	0.42
1:A:919:A:H2'	1:A:920:U:H6	1.85	0.42
12:L:93:LEU:O	12:L:96:VAL:HG23	2.19	0.42
10:J:62:HIS:O	14:N:58:LYS:HD2	2.19	0.42
1:A:309:G:C2	1:A:310:G:N7	2.87	0.42
1:A:684:A:C2	11:K:39:PRO:HG2	2.55	0.42
15:O:15:PHE:CE2	15:O:84:LYS:HG3	2.55	0.42
13:M:23:TYR:HB3	13:M:67:GLU:HA	2.02	0.42
7:G:76:ARG:HG3	7:G:156:TRP:HE1	1.85	0.42
2:B:20:GLU:HA	2:B:39:ILE:HG12	2.00	0.42
1:A:28:G:C6	1:A:29:G:N7	2.88	0.42
17:Q:37:LYS:O	17:Q:38:ARG:HD3	2.20	0.42
13:M:117:VAL:HB	13:M:118:ALA:H	1.63	0.42
1:A:1074:G:N2	1:A:1102:A:C4	2.88	0.42
1:A:1306:A:N3	1:A:1306:A:H2'	2.35	0.42
4:D:28:SER:CB	4:D:30:LYS:H	2.33	0.42
3:C:32:LEU:CD1	3:C:59:ARG:HE	2.33	0.42
6:F:78:GLU:O	6:F:81:ILE:HG13	2.20	0.42
1:A:235:C:H2'	1:A:236:G:C8	2.47	0.42
1:A:763:G:H2'	1:A:764:C:C6	2.54	0.42
18:R:76:LEU:O	18:R:78:LEU:HD12	2.20	0.42
1:A:522:C:H5"	1:A:523:A:OP2	2.20	0.42
1:A:702:A:HO2'	1:A:703:G:P	2.42	0.42
1:A:665:A:H2'	1:A:732:C:O2	2.20	0.42
1:A:976:G:OP2	14:N:32:SER:HA	2.20	0.42
13:M:15:VAL:HG23	13:M:43:THR:O	2.19	0.42
5:E:33:VAL:HG11	5:E:109:ILE:HA	2.00	0.42
1:A:1379:G:N7	7:G:2:ALA:HB3	2.35	0.42
1:A:945:G:C6	1:A:1337:G:C5	3.08	0.42
1:A:1248:A:C5	1:A:1249:C:C5	3.08	0.42
16:P:39:TYR:O	16:P:41:PRO:HD3	2.19	0.42
1:A:1054:C:O2'	22:A:1601:T1C:H922	2.20	0.42
19:S:32:LYS:HE2	19:S:57:HIS:CD2	2.55	0.42
1:A:1244:C:O2	1:A:1294:G:N2	2.53	0.42
15:O:2:PRO:O	15:O:3:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:33:GLN:H	10:J:33:GLN:HG2	1.51	0.42
1:A:667:G:O2'	15:O:51:HIS:HB2	2.20	0.42
1:A:1348:U:C5	1:A:1349:A:N7	2.88	0.42
1:A:515:G:C6	1:A:516:U:N3	2.87	0.42
1:A:964:A:O2'	10:J:55:LYS:HD2	2.20	0.42
1:A:578:C:O2'	1:A:728:A:H1'	2.19	0.42
1:A:373:A:N7	1:A:482:A:C8	2.88	0.42
9:I:113:LYS:H	9:I:119:ALA:HA	1.84	0.42
12:L:90:VAL:HG12	12:L:93:LEU:H	1.85	0.42
1:A:1096:C:H2'	1:A:1097:C:C6	2.55	0.42
5:E:99:GLY:H	5:E:117:ASP:CB	2.33	0.42
1:A:1125:U:O2'	1:A:1126:U:H2'	2.20	0.42
1:A:1511:G:H2'	1:A:1512:U:C6	2.54	0.42
17:Q:43:LEU:HD12	17:Q:68:ARG:HB2	2.02	0.42
1:A:496:A:H4'	1:A:497:A:O5'	2.18	0.42
8:H:2:LEU:HD12	8:H:3:THR:N	2.35	0.42
10:J:52:GLY:HA2	10:J:53:PRO:HD2	1.81	0.42
1:A:585:G:C6	1:A:586:C:C4	3.08	0.42
17:Q:7:THR:HA	17:Q:57:VAL:O	2.21	0.41
1:A:170:U:H2'	1:A:171:A:H8	1.85	0.41
5:E:94:ALA:HB1	5:E:98:THR:HB	2.01	0.41
8:H:44:PHE:O	8:H:80:ILE:HD11	2.20	0.41
6:F:53:ALA:O	6:F:55:ASP:N	2.45	0.41
1:A:1053:G:C4	1:A:1199:U:C5	3.07	0.41
1:A:613:C:C2	1:A:628:G:N2	2.88	0.41
8:H:34:GLU:HB3	8:H:118:VAL:HG11	2.02	0.41
1:A:293:G:H2'	1:A:294:U:C6	2.55	0.41
1:A:564:C:N1	17:Q:31:LEU:HD11	2.34	0.41
3:C:46:GLU:C	3:C:48:TYR:H	2.24	0.41
11:K:45:GLY:HA2	11:K:48:ILE:HG12	2.02	0.41
1:A:34:C:H42	1:A:550:G:H1	1.68	0.41
7:G:133:GLY:HA2	7:G:136:LYS:HD2	2.00	0.41
17:Q:16:GLN:HB3	17:Q:16:GLN:HE21	1.59	0.41
1:A:1034:G:H8	1:A:1034:G:O5'	2.02	0.41
1:A:1394:A:N6	1:A:1500:A:O2'	2.52	0.41
1:A:1367:C:OP2	9:I:112:LYS:NZ	2.49	0.41
1:A:481:G:HO2'	1:A:483:C:H41	1.58	0.41
1:A:1421:G:H2'	1:A:1422:G:O4'	2.20	0.41
8:H:21:LYS:O	8:H:63:LEU:HD12	2.20	0.41
1:A:689:C:OP2	11:K:46:GLY:HA3	2.18	0.41
3:C:152:ILE:HG22	3:C:154:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1250:A:H4'	9:I:67:GLY:HA2	2.01	0.41
1:A:995:C:N3	1:A:1046:A:O2'	2.49	0.41
1:A:36:C:O3'	12:L:123:LYS:HA	2.19	0.41
1:A:243:A:C2	1:A:245:C:N3	2.88	0.41
12:L:6:THR:HG23	12:L:9:GLN:HG3	2.02	0.41
18:R:44:LEU:O	18:R:51:LEU:HD11	2.20	0.41
6:F:98:LEU:HD22	6:F:98:LEU:HA	1.88	0.41
3:C:45:LYS:HE2	3:C:45:LYS:HB3	1.71	0.41
1:A:428:G:H4'	1:A:429:U:O5'	2.20	0.41
1:A:646:U:H6	1:A:646:U:O5'	2.03	0.41
1:A:376:G:C4	1:A:389:A:N1	2.88	0.41
1:A:1060:C:H5"	10:J:51:ARG:HB3	2.02	0.41
4:D:159:ARG:O	4:D:163:GLU:N	2.50	0.41
1:A:994:A:C8	1:A:1216:G:H4'	2.54	0.41
1:A:1454:G:O3'	20:T:35:THR:HG21	2.20	0.41
1:A:1527:C:C5	1:A:1528:U:C5	3.08	0.41
1:A:459:G:C2	1:A:474:G:O6	2.74	0.41
1:A:672:U:H5'	6:F:80:ARG:NH1	2.35	0.41
20:T:49:ALA:HB1	20:T:98:PRO:HA	2.02	0.41
1:A:705:U:H2'	1:A:706:A:C8	2.55	0.41
1:A:1351:U:O2'	1:A:1352:C:H5'	2.20	0.41
1:A:904:C:C4	1:A:905:U:C4	3.08	0.41
1:A:1347:G:O2'	1:A:1373:G:N1	2.29	0.41
1:A:1501:C:H5"	1:A:1502:A:OP2	2.20	0.41
1:A:1190:G:H5'	3:C:176:HIS:NE2	2.35	0.41
1:A:1151:A:O2'	1:A:1152:A:C8	2.73	0.41
5:E:94:ALA:HB3	5:E:118:ILE:N	2.34	0.41
5:E:78:HIS:O	5:E:93:PRO:HD3	2.20	0.41
1:A:977:A:H4'	1:A:977:A:OP2	2.20	0.41
1:A:402:G:C2'	1:A:403:C:H5'	2.50	0.41
1:A:655:A:N6	1:A:752:G:N2	2.69	0.41
2:B:74:LYS:O	2:B:77:ALA:N	2.51	0.41
5:E:9:LYS:H	5:E:112:LEU:CD1	2.33	0.41
1:A:727:G:C6	1:A:731:G:C6	3.08	0.41
1:A:684:A:N3	11:K:39:PRO:HG2	2.34	0.41
8:H:102:ARG:HG2	8:H:125:ARG:NH2	2.36	0.41
1:A:424:G:H2'	1:A:425:G:H8	1.85	0.41
1:A:1469:G:H2'	1:A:1470:G:C8	2.55	0.41
1:A:126:G:H4'	1:A:634:C:O2	2.21	0.41
6:F:3:ARG:HD3	6:F:3:ARG:HH11	1.75	0.41
1:A:1340:A:H2'	1:A:1341:U:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:81:LEU:O	13:M:89:GLY:HA3	2.21	0.41
10:J:27:ALA:O	10:J:32:ALA:HB3	2.20	0.41
1:A:1100:C:H5"	1:A:1101:A:OP2	2.20	0.41
8:H:109:ILE:HD12	8:H:110:ALA:H	1.85	0.41
1:A:720:C:OP2	1:A:721:G:H3'	2.20	0.41
1:A:1306:A:H3'	1:A:1307:U:C6	2.56	0.41
1:A:802:A:H2'	1:A:803:G:O4'	2.19	0.41
1:A:1206:G:C6	1:A:1207:G:C5	3.08	0.41
1:A:620:C:H2'	1:A:621:A:O4'	2.21	0.41
2:B:109:SER:O	2:B:112:VAL:HG23	2.20	0.41
5:E:78:HIS:HA	8:H:105:ARG:HB3	2.02	0.41
2:B:25:ASN:HA	2:B:26:PRO:HD3	1.78	0.41
1:A:988:G:N2	1:A:1218:C:O2	2.54	0.41
11:K:83:ILE:HD13	11:K:109:VAL:HB	2.01	0.41
1:A:146:G:H2'	1:A:147:G:C8	2.55	0.41
5:E:148:VAL:HG12	5:E:149:GLU:N	2.36	0.41
1:A:1035:A:H2'	1:A:1036:G:O4'	2.20	0.41
1:A:1071:C:OP1	5:E:27:ARG:NH1	2.52	0.41
1:A:739:C:C6	1:A:739:C:C3'	2.97	0.41
1:A:1055:A:C6	1:A:1206:G:C5	3.08	0.41
1:A:62:U:O2'	1:A:63:C:H5'	2.21	0.41
1:A:912:C:H5"	12:L:46:LYS:HZ1	1.85	0.41
1:A:836:G:C6	1:A:851:G:C6	3.09	0.41
1:A:1202:G:O4'	14:N:29:ARG:HD2	2.21	0.41
1:A:977:A:C8	1:A:1223:C:C4	3.08	0.41
3:C:174:PRO:HB2	3:C:177:THR:OG1	2.19	0.41
1:A:1225:A:OP2	1:A:1226:C:H5	2.04	0.41
10:J:62:HIS:HB3	14:N:59:ALA:HB3	2.01	0.41
7:G:26:PHE:HD1	7:G:101:LEU:HB3	1.85	0.41
8:H:97:VAL:HG23	8:H:98:LYS:N	2.35	0.41
1:A:278:G:OP2	17:Q:41:LYS:HD3	2.20	0.41
11:K:103:LEU:HA	11:K:103:LEU:HD23	1.89	0.41
1:A:981:U:H2'	1:A:982:U:C5	2.55	0.41
17:Q:16:GLN:C	17:Q:18:THR:H	2.23	0.41
19:S:11:VAL:HG13	19:S:15:LEU:HD23	2.02	0.41
1:A:1296:C:H5"	1:A:1297:C:OP2	2.20	0.41
1:A:796:C:H6	1:A:796:C:O5'	2.04	0.41
1:A:59:A:N3	1:A:59:A:H2'	2.36	0.41
1:A:407:G:C6	1:A:408:A:C6	3.09	0.41
1:A:673:G:C6	1:A:674:G:C6	3.08	0.41
15:O:63:ARG:NH1	15:O:87:ILE:HD13	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:G:C8	1:A:821:G:OP1	2.74	0.41
12:L:110:VAL:HG23	12:L:120:TYR:HB3	2.02	0.41
17:Q:63:ARG:HA	17:Q:64:PRO:HD2	1.67	0.41
1:A:1311:G:C2	1:A:1327:C:N3	2.89	0.41
5:E:78:HIS:HE1	5:E:80:ILE:HD12	1.86	0.41
1:A:921:U:H2'	1:A:922:G:O4'	2.21	0.41
13:M:113:PRO:O	13:M:115:LYS:NZ	2.54	0.41
1:A:1238:A:N3	1:A:1241:G:O2'	2.49	0.41
1:A:1301:U:C2	1:A:1303:C:C6	3.09	0.41
1:A:615:C:C4	1:A:616:G:N7	2.89	0.41
1:A:262:A:N1	1:A:263:A:C6	2.88	0.41
20:T:29:LYS:HZ3	20:T:66:ALA:HA	1.84	0.41
20:T:57:ARG:HD2	20:T:102:GLY:HA3	2.03	0.41
9:I:79:LEU:HD21	9:I:103:THR:O	2.21	0.41
1:A:188:C:H4'	20:T:89:ARG:NH1	2.36	0.41
16:P:21:VAL:HG11	16:P:59:TRP:CE3	2.55	0.41
1:A:1080:A:H5"	1:A:1081:G:OP2	2.21	0.41
1:A:1082:G:O2'	1:A:1083:U:H5'	2.20	0.41
1:A:17:U:O2'	1:A:1079:G:C2'	2.68	0.41
1:A:410:G:C2	1:A:429:U:C2	3.08	0.41
1:A:580:U:H2'	1:A:581:G:C8	2.56	0.41
4:D:19:LEU:HD22	4:D:67:ILE:HG12	2.03	0.41
17:Q:92:ARG:NH1	17:Q:95:TYR:HE2	2.16	0.41
1:A:701:C:H4'	1:A:703:G:C8	2.55	0.41
3:C:172:ARG:HB3	3:C:172:ARG:HE	1.44	0.41
1:A:834:C:C6	1:A:834:C:H3'	2.56	0.41
19:S:39:THR:HG23	19:S:70:LYS:NZ	2.36	0.41
1:A:1379:G:C6	1:A:1380:U:O4	2.73	0.41
1:A:134:A:C5	1:A:135:C:C4	3.09	0.41
5:E:31:LEU:HD12	5:E:31:LEU:HA	1.87	0.41
1:A:1077:G:C6	1:A:1081:G:C6	3.09	0.41
8:H:119:LEU:HD23	8:H:119:LEU:HA	1.76	0.41
1:A:1191:A:H2'	1:A:1192:C:C6	2.55	0.41
1:A:592:G:H2'	1:A:593:G:C8	2.56	0.41
4:D:10:ARG:HA	4:D:13:ARG:HG2	2.03	0.41
1:A:878:G:C6	1:A:879:C:N4	2.89	0.41
1:A:103:C:HO2'	1:A:172:A:H61	1.69	0.41
2:B:98:LEU:HB2	2:B:101:MET:HG3	2.02	0.41
2:B:105:PHE:HB2	2:B:158:LEU:HD21	2.03	0.41
5:E:115:VAL:HG11	5:E:118:ILE:HB	2.02	0.41
12:L:84:LEU:O	12:L:85:ILE:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:ILE:HG22	2:B:223:ILE:N	2.34	0.41
1:A:974:A:OP1	14:N:29:ARG:NH2	2.47	0.41
1:A:773:G:C2	1:A:807:A:C6	3.09	0.41
1:A:1517:G:C6	1:A:1518:A:C2	3.09	0.41
13:M:27:LYS:O	13:M:31:LYS:HG3	2.20	0.41
1:A:1014:A:H5'	19:S:33:THR:HG23	2.02	0.41
15:O:56:LEU:O	15:O:60:VAL:N	2.40	0.41
12:L:27:LEU:H	12:L:27:LEU:HG	1.61	0.41
3:C:164:ARG:HG2	3:C:164:ARG:H	1.64	0.41
1:A:1242:C:H2'	1:A:1243:C:O4'	2.21	0.41
5:E:43:LEU:O	5:E:62:ALA:HA	2.21	0.41
1:A:833:U:O5'	1:A:833:U:H6	2.03	0.41
1:A:829:G:H4'	2:B:24:TRP:HZ3	1.86	0.41
8:H:4:ASP:HA	8:H:5:PRO:HD2	1.87	0.41
5:E:18:ARG:HB3	5:E:19:MET:H	1.77	0.41
1:A:594:G:N1	1:A:646:U:O2	2.53	0.41
1:A:764:C:C4	1:A:765:G:N7	2.89	0.41
3:C:150:LYS:HG2	3:C:152:ILE:HD11	2.03	0.41
1:A:932:C:H2'	1:A:933:G:H8	1.81	0.41
7:G:26:PHE:O	7:G:29:LYS:N	2.54	0.41
1:A:715:A:O5'	1:A:715:A:H8	2.04	0.41
1:A:556:C:C2	1:A:557:G:C8	3.08	0.41
1:A:511:C:C2	1:A:512:U:C5	3.09	0.41
1:A:829:G:HO2'	2:B:24:TRP:HZ3	1.65	0.41
7:G:87:VAL:HG11	7:G:155:ARG:HA	2.02	0.41
7:G:39:ALA:HA	7:G:42:ILE:HB	2.03	0.41
13:M:106:ASN:N	13:M:106:ASN:OD1	2.54	0.41
5:E:89:ILE:HD12	5:E:89:ILE:HA	1.90	0.40
1:A:1266:G:C5	1:A:1268:A:OP2	2.75	0.40
1:A:370:C:H2'	1:A:371:G:C8	2.56	0.40
1:A:1187:G:H4'	9:I:111:ARG:NH1	2.36	0.40
4:D:92:VAL:HG12	4:D:96:LEU:HD11	2.03	0.40
2:B:112:VAL:O	2:B:115:LEU:N	2.45	0.40
12:L:89:ARG:HA	12:L:97:ARG:HA	2.03	0.40
1:A:1250:A:H2'	1:A:1251:A:C8	2.56	0.40
1:A:1238:A:H5"	1:A:1239:A:OP2	2.20	0.40
1:A:1355:G:H2'	1:A:1356:G:C8	2.57	0.40
1:A:1210:C:O4'	1:A:1214:C:N4	2.54	0.40
1:A:985:C:H2'	1:A:986:A:C8	2.56	0.40
1:A:302:G:O6	1:A:303:A:N6	2.54	0.40
1:A:814:A:O2'	1:A:815:A:H3'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:127:ASN:O	5:E:131:ILE:HG13	2.22	0.40
6:F:67:MET:HB2	6:F:67:MET:HE2	1.98	0.40
1:A:575:G:C2	1:A:821:G:C4	3.09	0.40
1:A:831:U:H4'	2:B:22:LYS:NZ	2.35	0.40
1:A:578:C:H1'	1:A:729:A:H1'	2.02	0.40
4:D:70:ILE:HG12	4:D:100:ARG:HE	1.86	0.40
5:E:76:ILE:HA	5:E:77:PRO:HD3	1.75	0.40
1:A:688:G:OP1	11:K:47:VAL:HG22	2.21	0.40
6:F:48:LEU:HD13	6:F:52:ILE:CG1	2.50	0.40
6:F:5:GLU:HG2	6:F:62:TRP:CZ2	2.55	0.40
6:F:5:GLU:HG2	6:F:62:TRP:HZ2	1.86	0.40
2:B:207:ALA:C	2:B:209:ARG:H	2.24	0.40
1:A:1358:U:H3'	1:A:1359:C:H6	1.86	0.40
1:A:1213:A:C4	1:A:1215:G:C5	3.09	0.40
1:A:1511:G:C5	1:A:1512:U:C5	3.09	0.40
15:O:22:THR:O	15:O:27:VAL:HG11	2.21	0.40
1:A:142:G:C2	1:A:143:A:N7	2.90	0.40
1:A:1316:G:H22	1:A:1319:A:H5"	1.86	0.40
1:A:20:U:O2'	1:A:21:G:H5'	2.21	0.40
16:P:39:TYR:CG	16:P:73:LEU:HD21	2.57	0.40
16:P:59:TRP:C	16:P:62:VAL:HB	2.41	0.40
1:A:287:U:O4	1:A:288:A:N6	2.54	0.40
19:S:40:ILE:HG13	19:S:40:ILE:H	1.61	0.40
5:E:130:ASN:O	5:E:134:ALA:N	2.41	0.40
1:A:430:A:H2'	1:A:431:A:O4'	2.21	0.40
1:A:880:C:H2'	1:A:881:G:C8	2.56	0.40
12:L:102:ARG:NH2	12:L:108:ALA:HB3	2.34	0.40
1:A:592:G:H2'	1:A:593:G:H8	1.86	0.40
1:A:728:A:H2'	1:A:729:A:H8	1.85	0.40
1:A:578:C:C1'	1:A:729:A:H1'	2.51	0.40
1:A:370:C:O2'	1:A:371:G:H5'	2.21	0.40
1:A:1159:U:H4'	1:A:1160:G:OP1	2.21	0.40
1:A:689:C:H2'	1:A:690:G:O4'	2.21	0.40
1:A:701:C:H4'	1:A:702:A:H5'	2.02	0.40
1:A:1111:A:N1	3:C:177:THR:HG23	2.37	0.40
1:A:1251:A:N3	1:A:1369:C:O2'	2.53	0.40
1:A:665:A:C2	1:A:732:C:C5	3.10	0.40
2:B:11:LEU:HD23	2:B:16:HIS:HD2	1.87	0.40
1:A:300:A:H8	1:A:300:A:O5'	2.04	0.40
1:A:986:A:C4	1:A:1220:G:N2	2.90	0.40
1:A:134:A:C4	1:A:325:A:C2	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:G:C2	1:A:148:G:C5	3.09	0.40
3:C:8:ILE:HG23	3:C:16:ARG:HE	1.85	0.40
1:A:35:G:C2	1:A:550:G:N3	2.89	0.40
7:G:23:VAL:HG13	7:G:43:PHE:CE2	2.56	0.40
1:A:364:A:H2'	1:A:365:U:O2	2.20	0.40
5:E:133:TYR:HA	5:E:136:MET:HB2	2.03	0.40
4:D:156:GLU:HG3	4:D:157:LEU:H	1.86	0.40
1:A:669:U:H3	1:A:737:A:N6	2.13	0.40
16:P:79:VAL:HG12	16:P:80:PHE:CD1	2.57	0.40
1:A:983:A:C2	1:A:984:C:C6	3.09	0.40
1:A:136:C:O2'	1:A:137:C:H5'	2.22	0.40
6:F:11:ASN:OD1	6:F:11:ASN:N	2.52	0.40
15:O:50:HIS:O	15:O:53:HIS:HB3	2.21	0.40
4:D:21:LEU:CD2	4:D:114:ARG:HB2	2.52	0.40
1:A:192:U:H5"	20:T:57:ARG:HH21	1.87	0.40
1:A:1088:G:C4	1:A:1089:G:C8	3.10	0.40
1:A:282:A:OP2	1:A:283:C:H5	2.03	0.40
5:E:122:GLU:O	5:E:123:LEU:HG	2.21	0.40
3:C:130:VAL:O	3:C:133:ALA:HB3	2.21	0.40
1:A:752:G:H4'	1:A:754:C:C5	2.52	0.40
20:T:33:ILE:HD11	20:T:62:LEU:HB3	2.03	0.40
1:A:414:A:H2'	1:A:415:A:C8	2.57	0.40
5:E:7:GLU:HG3	5:E:8:GLU:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	224/226 (99%)	154 (69%)	45 (20%)	25 (11%)	0 7
3	C	204/206 (99%)	142 (70%)	45 (22%)	17 (8%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	206/208 (99%)	147 (71%)	34 (16%)	25 (12%)	0 6
5	E	155/157 (99%)	109 (70%)	30 (19%)	16 (10%)	1 8
6	F	99/101 (98%)	79 (80%)	11 (11%)	9 (9%)	1 10
7	G	153/155 (99%)	113 (74%)	32 (21%)	8 (5%)	2 24
8	H	136/138 (99%)	98 (72%)	26 (19%)	12 (9%)	1 11
9	I	125/127 (98%)	96 (77%)	23 (18%)	6 (5%)	3 27
10	J	97/99 (98%)	78 (80%)	15 (16%)	4 (4%)	3 32
11	K	113/115 (98%)	90 (80%)	16 (14%)	7 (6%)	2 19
12	L	122/124 (98%)	85 (70%)	28 (23%)	9 (7%)	1 15
13	M	117/119 (98%)	90 (77%)	19 (16%)	8 (7%)	1 17
14	N	58/60 (97%)	47 (81%)	10 (17%)	1 (2%)	11 52
15	O	86/88 (98%)	63 (73%)	21 (24%)	2 (2%)	8 46
16	P	83/85 (98%)	60 (72%)	20 (24%)	3 (4%)	4 36
17	Q	102/104 (98%)	78 (76%)	14 (14%)	10 (10%)	1 9
18	R	71/73 (97%)	49 (69%)	15 (21%)	7 (10%)	1 9
19	S	81/83 (98%)	66 (82%)	11 (14%)	4 (5%)	3 26
20	T	97/99 (98%)	74 (76%)	18 (19%)	5 (5%)	2 24
21	V	22/24 (92%)	18 (82%)	2 (9%)	2 (9%)	1 10
All	All	2351/2391 (98%)	1736 (74%)	435 (18%)	180 (8%)	1 14

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	29	ALA
2	B	30	ARG
2	B	78	GLN
2	B	82	ARG
2	B	101	MET
2	B	104	ASN
2	B	150	SER
2	B	166	ASP
2	B	181	PHE
3	C	12	LEU
3	C	45	LYS
3	C	47	LEU
3	C	157	ILE

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Mol	Chain	Res	Type
3	C	167	TRP
4	D	40	PRO
4	D	42	GLN
4	D	44	GLY
4	D	95	GLY
4	D	110	PHE
4	D	163	GLU
4	D	164	ALA
4	D	170	VAL
4	D	172	PRO
4	D	178	VAL
4	D	193	ASP
5	E	37	ARG
5	E	41	VAL
5	E	100	VAL
5	E	145	LYS
5	E	152	ARG
5	E	153	LYS
6	F	4	TYR
6	F	34	GLY
6	F	48	LEU
6	F	54	LYS
7	G	3	ARG
7	G	35	LYS
7	G	55	GLY
8	H	18	ARG
8	H	43	GLY
8	H	76	PRO
8	H	91	ARG
9	I	38	GLN
9	I	117	HIS
10	J	41	PRO
10	J	90	LEU
11	K	35	PRO
11	K	106	LYS
11	K	124	LYS
12	L	52	LEU
12	L	106	ASP
13	M	48	LEU
16	P	31	LYS
17	Q	14	LYS
17	Q	16	GLN

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Mol	Chain	Res	Type
17	Q	30	PRO
17	Q	94	ASN
17	Q	98	LEU
18	R	37	VAL
18	R	66	LEU
18	R	77	GLY
2	B	17	PHE
2	B	37	ASN
2	B	75	LYS
2	B	89	GLY
2	B	177	ALA
2	B	227	GLY
3	C	88	ARG
3	C	107	GLN
3	C	179	ARG
3	C	188	LEU
4	D	7	PRO
4	D	29	PRO
4	D	41	GLY
4	D	55	ALA
4	D	56	VAL
4	D	84	LYS
4	D	106	TYR
4	D	137	SER
5	E	22	GLY
5	E	23	GLY
5	E	34	VAL
5	E	99	GLY
6	F	16	GLN
6	F	17	SER
6	F	23	LYS
6	F	65	VAL
7	G	24	THR
8	H	19	VAL
8	H	28	ALA
8	H	79	VAL
9	I	119	ALA
10	J	82	ILE
12	L	25	PRO
12	L	28	LYS
12	L	46	LYS
13	M	82	MET

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Mol	Chain	Res	Type
15	O	67	LEU
17	Q	47	PRO
17	Q	80	GLY
19	S	8	GLY
19	S	54	GLY
19	S	64	GLU
21	V	9	ARG
2	B	52	GLU
3	C	44	GLU
3	C	171	GLY
3	C	189	ALA
4	D	28	SER
4	D	117	ALA
4	D	194	LEU
5	E	104	ALA
5	E	154	GLY
8	H	27	PRO
8	H	68	ARG
8	H	96	GLY
10	J	36	GLY
11	K	15	ALA
11	K	39	PRO
12	L	51	ALA
13	M	67	GLU
13	M	104	ARG
17	Q	50	LYS
18	R	59	SER
19	S	65	ASN
20	T	10	LEU
20	T	95	ALA
20	T	102	GLY
2	B	65	GLY
2	B	147	LYS
2	B	196	LEU
3	C	9	GLY
3	C	61	ALA
3	C	169	ALA
4	D	10	ARG
5	E	27	ARG
5	E	102	ALA
6	F	53	ALA
7	G	77	SER

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Mol	Chain	Res	Type
7	G	81	GLY
7	G	123	GLU
9	I	105	ASP
12	L	73	GLU
12	L	125	PRO
13	M	12	ASN
14	N	35	ARG
15	O	27	VAL
17	Q	43	LEU
18	R	19	LYS
18	R	73	ALA
2	B	83	MET
2	B	216	SER
4	D	63	LYS
8	H	67	PRO
11	K	65	ALA
11	K	117	ASN
12	L	31	PRO
13	M	10	PRO
13	M	21	TYR
16	P	28	ARG
17	Q	97	SER
18	R	53	ARG
20	T	94	ALA
2	B	38	GLY
3	C	81	GLY
8	H	74	PRO
2	B	211	ILE
5	E	92	LYS
5	E	96	PRO
9	I	53	VAL
9	I	97	LYS
4	D	197	PRO
2	B	208	ILE
3	C	197	GLY
7	G	130	GLY
16	P	79	VAL
21	V	13	ILE
13	M	117	VAL
20	T	63	ILE
2	B	91	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	195/195 (100%)	147 (75%)	48 (25%)	1	4
3	C	160/160 (100%)	130 (81%)	30 (19%)	2	9
4	D	180/180 (100%)	139 (77%)	41 (23%)	1	5
5	E	119/119 (100%)	85 (71%)	34 (29%)	0	3
6	F	90/90 (100%)	60 (67%)	30 (33%)	0	2
7	G	126/126 (100%)	109 (86%)	17 (14%)	5	25
8	H	119/119 (100%)	90 (76%)	29 (24%)	1	4
9	I	98/98 (100%)	79 (81%)	19 (19%)	2	8
10	J	89/89 (100%)	79 (89%)	10 (11%)	7	33
11	K	87/87 (100%)	70 (80%)	17 (20%)	2	8
12	L	104/104 (100%)	87 (84%)	17 (16%)	3	16
13	M	95/95 (100%)	78 (82%)	17 (18%)	2	11
14	N	49/49 (100%)	35 (71%)	14 (29%)	0	3
15	O	79/79 (100%)	62 (78%)	17 (22%)	1	6
16	P	73/73 (100%)	58 (80%)	15 (20%)	1	7
17	Q	96/96 (100%)	78 (81%)	18 (19%)	2	9
18	R	64/64 (100%)	49 (77%)	15 (23%)	1	4
19	S	72/72 (100%)	60 (83%)	12 (17%)	3	15
20	T	76/76 (100%)	64 (84%)	12 (16%)	3	18
21	V	19/19 (100%)	12 (63%)	7 (37%)	0	2
All	All	1990/1990 (100%)	1571 (79%)	419 (21%)	1	6

All (419) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	3	VAL
2	B	6	THR
2	B	7	VAL

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Mol	Chain	Res	Type
2	B	9	GLU
2	B	17	PHE
2	B	19	HIS
2	B	33	TYR
2	B	41	ILE
2	B	42	ILE
2	B	47	THR
2	B	51	LEU
2	B	53	ARG
2	B	60	ASP
2	B	61	LEU
2	B	71	VAL
2	B	75	LYS
2	B	83	MET
2	B	94	ASN
2	B	95	GLN
2	B	96	ARG
2	B	103	THR
2	B	112	VAL
2	B	115	LEU
2	B	118	LEU
2	B	121	LEU
2	B	124	SER
2	B	126	GLU
2	B	127	ILE
2	B	137	ARG
2	B	138	LEU
2	B	139	LYS
2	B	144	ARG
2	B	145	LEU
2	B	152	PHE
2	B	153	ARG
2	B	155	LEU
2	B	157	ARG
2	B	164	VAL
2	B	178	ARG
2	B	180	LEU
2	B	181	PHE
2	B	190	THR
2	B	196	LEU
2	B	198	ASP
2	B	205	ASP

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Mol	Chain	Res	Type
2	B	208	ILE
2	B	216	SER
2	B	224	GLN
3	C	3	ASN
3	C	4	LYS
3	C	5	ILE
3	C	20	SER
3	C	21	ARG
3	C	22	TRP
3	C	27	LYS
3	C	32	LEU
3	C	34	LEU
3	C	43	LEU
3	C	56	ASP
3	C	59	ARG
3	C	83	ARG
3	C	94	LEU
3	C	95	THR
3	C	97	LYS
3	C	98	ASN
3	C	103	VAL
3	C	127	ARG
3	C	134	ILE
3	C	142	MET
3	C	164	ARG
3	C	167	TRP
3	C	170	GLN
3	C	172	ARG
3	C	177	THR
3	C	191	THR
3	C	192	THR
3	C	204	LEU
3	C	207	VAL
4	D	5	ILE
4	D	9	CYS
4	D	10	ARG
4	D	11	LEU
4	D	12	CYS
4	D	13	ARG
4	D	15	GLU
4	D	17	VAL
4	D	18	LYS

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Mol	Chain	Res	Type
4	D	26	CYS
4	D	28	SER
4	D	36	ARG
4	D	47	ARG
4	D	49	ARG
4	D	53	ASP
4	D	57	ARG
4	D	59	ARG
4	D	60	GLU
4	D	67	ILE
4	D	73	ARG
4	D	76	ARG
4	D	96	LEU
4	D	103	ASN
4	D	108	LEU
4	D	110	PHE
4	D	122	ARG
4	D	141	ARG
4	D	145	GLU
4	D	148	VAL
4	D	152	SER
4	D	154	ASN
4	D	155	LEU
4	D	160	GLN
4	D	162	LEU
4	D	170	VAL
4	D	178	VAL
4	D	179	GLU
4	D	184	LYS
4	D	187	ARG
4	D	194	LEU
4	D	202	LEU
5	E	6	PHE
5	E	7	GLU
5	E	9	LYS
5	E	13	ILE
5	E	18	ARG
5	E	24	ARG
5	E	25	ARG
5	E	26	PHE
5	E	33	VAL
5	E	38	GLN

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Mol	Chain	Res	Type
5	E	40	ARG
5	E	43	LEU
5	E	53	LEU
5	E	57	LYS
5	E	60	TYR
5	E	64	ARG
5	E	68	GLU
5	E	75	THR
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	84	PHE
5	E	98	THR
5	E	107	ARG
5	E	112	LEU
5	E	116	THR
5	E	119	LEU
5	E	129	ILE
5	E	131	ILE
5	E	133	TYR
5	E	135	THR
5	E	142	LEU
5	E	149	GLU
5	E	155	GLU
6	F	3	ARG
6	F	4	TYR
6	F	8	ILE
6	F	10	LEU
6	F	13	ASN
6	F	18	GLN
6	F	19	LEU
6	F	21	LEU
6	F	25	ILE
6	F	28	ARG
6	F	32	ASN
6	F	36	ARG
6	F	45	LEU
6	F	54	LYS
6	F	55	ASP
6	F	61	LEU
6	F	66	GLU
6	F	67	MET

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Mol	Chain	Res	Type
6	F	69	GLU
6	F	70	ASP
6	F	75	LEU
6	F	77	ARG
6	F	79	LEU
6	F	81	ILE
6	F	82	ARG
6	F	88	VAL
6	F	90	VAL
6	F	95	GLU
6	F	98	LEU
6	F	100	ASN
7	G	3	ARG
7	G	4	ARG
7	G	5	ARG
7	G	8	GLU
7	G	36	LYS
7	G	84	ASN
7	G	89	MET
7	G	92	SER
7	G	98	SER
7	G	115	ARG
7	G	118	VAL
7	G	124	LEU
7	G	138	LYS
7	G	149	ARG
7	G	151	TYR
7	G	155	ARG
7	G	156	TRP
8	H	1	MET
8	H	3	THR
8	H	13	ILE
8	H	14	ARG
8	H	18	ARG
8	H	24	THR
8	H	31	PHE
8	H	36	LEU
8	H	37	ARG
8	H	39	LEU
8	H	58	TYR
8	H	60	ARG
8	H	68	ARG

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Mol	Chain	Res	Type
8	H	73	ASP
8	H	78	GLN
8	H	80	ILE
8	H	86	ILE
8	H	91	ARG
8	H	97	VAL
8	H	104	ARG
8	H	109	ILE
8	H	111	ILE
8	H	112	LEU
8	H	118	VAL
8	H	122	ARG
8	H	125	ARG
8	H	126	LYS
8	H	129	VAL
8	H	137	VAL
9	I	3	GLN
9	I	7	THR
9	I	9	ARG
9	I	14	VAL
9	I	16	ARG
9	I	27	THR
9	I	32	ASP
9	I	33	PHE
9	I	34	ASN
9	I	50	LEU
9	I	53	VAL
9	I	91	ASP
9	I	93	ARG
9	I	97	LYS
9	I	99	LEU
9	I	104	ARG
9	I	108	VAL
9	I	113	LYS
9	I	121	ARG
10	J	16	LEU
10	J	17	ASP
10	J	24	VAL
10	J	28	ARG
10	J	33	GLN
10	J	40	LEU
10	J	54	PHE

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Mol	Chain	Res	Type
10	J	65	LEU
10	J	74	ILE
10	J	92	THR
11	K	16	SER
11	K	26	ASN
11	K	30	VAL
11	K	34	ASP
11	K	47	VAL
11	K	51	LYS
11	K	63	LEU
11	K	66	LEU
11	K	70	LYS
11	K	80	VAL
11	K	81	ASP
11	K	82	VAL
11	K	96	ARG
11	K	99	GLN
11	K	106	LYS
11	K	109	VAL
11	K	120	ARG
12	L	7	ILE
12	L	18	VAL
12	L	22	SER
12	L	46	LYS
12	L	50	SER
12	L	55	VAL
12	L	62	SER
12	L	81	SER
12	L	92	ASP
12	L	93	LEU
12	L	96	VAL
12	L	97	ARG
12	L	98	TYR
12	L	110	VAL
12	L	111	LYS
12	L	112	ASP
12	L	118	SER
13	M	11	ARG
13	M	16	ASP
13	M	17	VAL
13	M	19	LEU
13	M	32	GLU

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Mol	Chain	Res	Type
13	M	39	ILE
13	M	44	ARG
13	M	54	VAL
13	M	63	THR
13	M	66	LEU
13	M	79	LYS
13	M	101	GLN
13	M	106	ASN
13	M	108	ARG
13	M	109	THR
13	M	117	VAL
13	M	120	LYS
14	N	13	THR
14	N	15	LYS
14	N	16	PHE
14	N	17	LYS
14	N	18	VAL
14	N	25	VAL
14	N	31	ARG
14	N	35	ARG
14	N	40	CYS
14	N	44	LEU
14	N	46	GLU
14	N	53	LEU
14	N	56	VAL
14	N	58	LYS
15	O	7	GLU
15	O	15	PHE
15	O	17	ARG
15	O	18	PHE
15	O	22	THR
15	O	25	THR
15	O	32	LEU
15	O	40	SER
15	O	47	LYS
15	O	53	HIS
15	O	57	LEU
15	O	66	LEU
15	O	67	LEU
15	O	68	ARG
15	O	70	LEU
15	O	79	ARG

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Mol	Chain	Res	Type
15	O	87	ILE
16	P	1	MET
16	P	4	ILE
16	P	8	ARG
16	P	14	ASN
16	P	32	TYR
16	P	33	ILE
16	P	36	ILE
16	P	38	TYR
16	P	45	THR
16	P	54	GLU
16	P	60	LEU
16	P	65	GLN
16	P	67	THR
16	P	73	LEU
16	P	85	ARG
17	Q	7	THR
17	Q	16	GLN
17	Q	18	THR
17	Q	19	VAL
17	Q	25	ARG
17	Q	28	PRO
17	Q	34	LYS
17	Q	37	LYS
17	Q	38	ARG
17	Q	39	SER
17	Q	48	GLU
17	Q	49	GLU
17	Q	50	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	72	ARG
17	Q	83	ASP
17	Q	98	LEU
18	R	25	THR
18	R	34	TYR
18	R	35	ARG
18	R	36	ASN
18	R	40	LEU
18	R	50	ILE
18	R	53	ARG
18	R	56	THR

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Mol	Chain	Res	Type
18	R	58	LEU
18	R	68	LYS
18	R	69	THR
18	R	74	ARG
18	R	75	ILE
18	R	82	THR
18	R	87	ARG
19	S	3	ARG
19	S	4	SER
19	S	15	LEU
19	S	28	LYS
19	S	37	ARG
19	S	39	THR
19	S	41	VAL
19	S	43	GLU
19	S	53	ASN
19	S	71	LEU
19	S	78	ARG
19	S	79	THR
20	T	18	GLN
20	T	19	SER
20	T	36	LEU
20	T	37	SER
20	T	45	GLN
20	T	50	GLU
20	T	56	MET
20	T	62	LEU
20	T	70	SER
20	T	71	THR
20	T	83	ARG
20	T	91	LEU
21	V	3	LYS
21	V	6	ARG
21	V	8	THR
21	V	9	ARG
21	V	10	ARG
21	V	12	LYS
21	V	13	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	16	HIS
4	D	116	GLN
4	D	123	HIS
4	D	125	HIS
9	I	38	GLN
9	I	73	GLN
10	J	33	GLN
10	J	56	HIS
12	L	49	ASN
12	L	99	HIS
15	O	46	HIS
15	O	62	GLN
19	S	47	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1507 (99%)	396 (26%)	7 (0%)

All (396) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	7	G
1	A	8	A
1	A	9	G
1	A	10	A
1	A	14	U
1	A	19	C
1	A	25	C
1	A	27	G
1	A	30	U
1	A	31	G
1	A	32	A
1	A	39	G
1	A	40	C
1	A	44	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	51	A
1	A	61	G

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Mol	Chain	Res	Type
1	A	64	G
1	A	66	G
1	A	69	G
1	A	84	U
1	A	88	A
1	A	93	G
1	A	98	U
1	A	101	A
1	A	108	G
1	A	115	G
1	A	116	A
1	A	117	G
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	146	G
1	A	149	A
1	A	163	C
1	A	182	U
1	A	183	G
1	A	190(B)	C
1	A	190(C)	C
1	A	190(I)	G
1	A	195	A
1	A	197	A
1	A	199	G
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	217	C
1	A	220	G
1	A	226	G
1	A	228	A
1	A	240	C
1	A	241	C
1	A	243	A
1	A	247	G
1	A	248	C
1	A	251	G

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Mol	Chain	Res	Type
1	A	253	U
1	A	266	G
1	A	267	C
1	A	279	A
1	A	280	C
1	A	281	G
1	A	289	G
1	A	293	G
1	A	298	A
1	A	301	G
1	A	305	G
1	A	306	G
1	A	308	C
1	A	314	C
1	A	319	G
1	A	321	A
1	A	328	C
1	A	330	C
1	A	332	G
1	A	345	C
1	A	346	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	357	G
1	A	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	384	G
1	A	397	A
1	A	398	C
1	A	403	C
1	A	406	G
1	A	410	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	418	C
1	A	421	U
1	A	422	C

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Mol	Chain	Res	Type
1	A	424	G
1	A	427	U
1	A	429	U
1	A	430	A
1	A	433	C
1	A	439	A
1	A	440	A
1	A	448	A
1	A	452	A
1	A	453	A
1	A	460	A
1	A	461	C
1	A	462	G
1	A	480	U
1	A	481	G
1	A	482	A
1	A	483	C
1	A	484	G
1	A	486	U
1	A	497	A
1	A	498	U
1	A	500	G
1	A	501	C
1	A	505	G
1	A	507	C
1	A	511	C
1	A	514	C
1	A	518	C
1	A	522	C
1	A	523	A
1	A	524	G
1	A	527	G
1	A	531	U
1	A	533	A
1	A	545	C
1	A	546	G
1	A	547	A
1	A	548	G
1	A	558	G
1	A	559	A
1	A	560	U
1	A	561	U

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Mol	Chain	Res	Type
1	A	562	C
1	A	564	C
1	A	567	G
1	A	570	G
1	A	572	A
1	A	573	A
1	A	574	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	596	C
1	A	597	G
1	A	605	U
1	A	606	G
1	A	623	C
1	A	642	A
1	A	652	U
1	A	653	A
1	A	665	A
1	A	666	G
1	A	667	G
1	A	669	U
1	A	671	G
1	A	678	U
1	A	687	A
1	A	688	G
1	A	694	A
1	A	695	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	716	A
1	A	720	C
1	A	721	G
1	A	723	U
1	A	724	G
1	A	728	A
1	A	730	G
1	A	731	G
1	A	741	G
1	A	750	G
1	A	755	G

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Mol	Chain	Res	Type
1	A	758	G
1	A	759	A
1	A	774	G
1	A	777	A
1	A	787	A
1	A	793	U
1	A	794	A
1	A	800	G
1	A	805	C
1	A	809	G
1	A	813	U
1	A	814	A
1	A	815	A
1	A	816	A
1	A	817	C
1	A	818	G
1	A	820	U
1	A	821	G
1	A	822	C
1	A	823	G
1	A	829	G
1	A	831	U
1	A	836	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	852	G
1	A	864	A
1	A	869	G
1	A	870	U
1	A	873	A
1	A	884	U
1	A	888	G
1	A	902	G
1	A	907	A
1	A	913	A
1	A	914	A
1	A	916	G
1	A	918	A
1	A	922	G
1	A	926	G

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Mol	Chain	Res	Type
1	A	927	G
1	A	928	G
1	A	934	C
1	A	936	C
1	A	939	G
1	A	951	G
1	A	955	U
1	A	960	U
1	A	961	U
1	A	966	G
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	980	C
1	A	987	G
1	A	988	G
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1016	A
1	A	1020	U
1	A	1025	U
1	A	1026	G
1	A	1032	G
1	A	1045	C
1	A	1050	G
1	A	1053	G
1	A	1065	U
1	A	1066	C
1	A	1076	C
1	A	1077	G
1	A	1078	U
1	A	1079	G
1	A	1081	G
1	A	1087	G
1	A	1094	G
1	A	1095	U

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Mol	Chain	Res	Type
1	A	1099	G
1	A	1100	C
1	A	1101	A
1	A	1102	A
1	A	1106	G
1	A	1129	C
1	A	1136	U
1	A	1137	C
1	A	1139	G
1	A	1141	C
1	A	1146	A
1	A	1151	A
1	A	1152	A
1	A	1153	C
1	A	1154	G
1	A	1159	U
1	A	1160	G
1	A	1167	A
1	A	1171	G
1	A	1175	G
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1218	C
1	A	1224	G
1	A	1225	A
1	A	1227	A
1	A	1228	C
1	A	1236	A
1	A	1238	A
1	A	1239	A
1	A	1240	U
1	A	1241	G
1	A	1245	A
1	A	1248	A

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Mol	Chain	Res	Type
1	A	1252	A
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1262	C
1	A	1267	C
1	A	1268	A
1	A	1270	C
1	A	1278	U
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1287	A
1	A	1289	A
1	A	1300	G
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1306	A
1	A	1308	U
1	A	1312	G
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1321	C
1	A	1322	C
1	A	1323	G
1	A	1335	C
1	A	1336	C
1	A	1337	G
1	A	1338	G
1	A	1346	A
1	A	1350	A
1	A	1353	G
1	A	1360	A
1	A	1362	C
1	A	1363	A
1	A	1370	G
1	A	1376	U
1	A	1380	U

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Mol	Chain	Res	Type
1	A	1391	U
1	A	1394	A
1	A	1397	C
1	A	1398	A
1	A	1400	C
1	A	1402	C
1	A	1410	G
1	A	1411	C
1	A	1416	G
1	A	1417	G
1	A	1418	A
1	A	1425	U
1	A	1442	G
1	A	1443	G
1	A	1451	A
1	A	1452	C
1	A	1453	G
1	A	1454	G
1	A	1466	C
1	A	1475	G
1	A	1480	G
1	A	1491	G
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1506	U
1	A	1513	A
1	A	1517	G
1	A	1518	A
1	A	1519	A
1	A	1520	G
1	A	1525	G
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	481	G
1	A	496	A
1	A	702	A
1	A	793	U
1	A	1145	C
1	A	1183	A
1	A	1529	G

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 106 ligands modelled in this entry, 105 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	T1C	A	1601	23	44,45,45	1.50	5 (11%)	48,72,72	0.85	1 (2%)

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
22	T1C	A	1601	23	-	0/22/80/80	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	T1C	C7-N7	2.52	1.49	1.42
22	A	1601	T1C	C4-C3	3.15	1.58	1.51
22	A	1601	T1C	C4-N4	3.88	1.55	1.47
22	A	1601	T1C	C8-C7	4.10	1.46	1.39
22	A	1601	T1C	C41-C4	5.42	1.60	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	1601	T1C	C41-C1C-C1	2.73	114.27	111.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	T1C	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1507/1507 (100%)	-0.62	5 (0%) 94 92	141, 212, 294, 438	0
2	B	226/226 (100%)	-0.00	14 (6%) 24 22	113, 192, 235, 265	0
3	C	206/206 (100%)	-0.45	3 (1%) 76 71	137, 204, 238, 266	0
4	D	208/208 (100%)	0.27	12 (5%) 26 24	125, 184, 221, 235	0
5	E	157/157 (100%)	0.58	21 (13%) 4 5	115, 165, 225, 272	0
6	F	101/101 (100%)	-0.10	5 (4%) 32 28	136, 190, 228, 264	0
7	G	155/155 (100%)	-0.18	8 (5%) 31 27	162, 226, 265, 299	0
8	H	138/138 (100%)	-0.00	4 (2%) 55 49	104, 167, 200, 223	0
9	I	127/127 (100%)	0.11	8 (6%) 23 21	144, 230, 273, 295	0
10	J	99/99 (100%)	0.83	18 (18%) 2 2	159, 222, 278, 287	0
11	K	115/115 (100%)	0.28	9 (7%) 16 15	155, 210, 239, 245	0
12	L	124/124 (100%)	0.92	24 (19%) 1 2	139, 201, 228, 293	0
13	M	119/119 (100%)	0.96	29 (24%) 1 1	194, 235, 259, 271	0
14	N	60/60 (100%)	0.26	2 (3%) 50 45	156, 212, 240, 247	0
15	O	88/88 (100%)	-0.40	0 100 100	107, 185, 225, 256	0
16	P	85/85 (100%)	0.76	11 (12%) 5 5	156, 198, 238, 282	0
17	Q	104/104 (100%)	1.26	34 (32%) 1 0	147, 196, 234, 331	0
18	R	73/73 (100%)	1.30	18 (24%) 1 1	121, 187, 281, 319	0
19	S	83/83 (100%)	0.44	10 (12%) 6 7	168, 250, 281, 295	0
20	T	99/99 (100%)	0.50	11 (11%) 7 7	184, 219, 267, 292	0
21	V	24/24 (100%)	0.96	5 (20%) 1 1	178, 205, 231, 244	0
All	All	3898/3898 (100%)	-0.05	251 (6%) 23 21	104, 206, 274, 438	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Q	105	ALA	11.8
17	Q	104	LYS	11.7
17	Q	103	GLY	10.3
10	J	35	SER	9.0
10	J	34	VAL	8.7
12	L	128	ALA	8.7
11	K	86	GLY	8.2
13	M	45	VAL	8.1
12	L	32	PHE	8.0
11	K	23	ALA	7.4
9	I	9	ARG	6.3
12	L	127	GLU	6.3
18	R	22	VAL	6.2
21	V	2	GLY	6.2
18	R	19	LYS	5.9
11	K	87	THR	5.5
12	L	68	ALA	5.5
12	L	70	ILE	5.3
13	M	2	ALA	5.1
5	E	118	ILE	5.1
16	P	17	TYR	5.0
10	J	73	ASP	5.0
5	E	89	ILE	5.0
10	J	39	PRO	4.9
18	R	20	ALA	4.9
10	J	71	LEU	4.9
18	R	16	PRO	4.9
12	L	112	ASP	4.9
8	H	54	ASP	4.8
12	L	30	ALA	4.8
5	E	91	LEU	4.8
3	C	193	TYR	4.8
11	K	50	TYR	4.7
10	J	36	GLY	4.7
10	J	37	PRO	4.7
18	R	18	ARG	4.7
5	E	19	MET	4.7
9	I	7	THR	4.7
13	M	5	ALA	4.6
5	E	22	GLY	4.6
18	R	17	SER	4.5
17	Q	8	GLY	4.5
18	R	31	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
18	R	23	LYS	4.4
13	M	9	ILE	4.4
6	F	101	ALA	4.4
13	M	10	PRO	4.3
12	L	69	TYR	4.3
13	M	119	GLY	4.3
7	G	84	ASN	4.2
20	T	10	LEU	4.1
10	J	72	VAL	4.1
12	L	33	ARG	4.0
17	Q	42	TYR	4.0
17	Q	44	ALA	4.0
12	L	31	PRO	3.9
1	A	82	U	3.9
9	I	8	GLY	3.9
17	Q	64	PRO	3.9
13	M	13	LYS	3.9
2	B	134	GLU	3.9
13	M	16	ASP	3.9
19	S	31	ILE	3.9
10	J	38	ILE	3.8
8	H	1	MET	3.8
16	P	56	ALA	3.8
4	D	134	ASP	3.7
17	Q	71	PHE	3.7
19	S	11	VAL	3.7
18	R	43	PHE	3.7
13	M	42	ALA	3.7
13	M	4	ILE	3.7
4	D	147	ALA	3.7
12	L	85	ILE	3.6
5	E	21	ALA	3.6
17	Q	43	LEU	3.6
2	B	131	PRO	3.6
5	E	30	ALA	3.6
13	M	43	THR	3.6
13	M	21	TYR	3.6
5	E	23	GLY	3.6
19	S	32	LYS	3.6
20	T	9	ASN	3.6
9	I	128	ARG	3.5
5	E	20	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
12	L	71	PRO	3.4
12	L	100	ILE	3.4
7	G	85	TYR	3.4
4	D	133	VAL	3.4
13	M	17	VAL	3.4
2	B	148	TYR	3.4
18	R	21	LYS	3.4
5	E	45	PHE	3.4
20	T	11	SER	3.3
2	B	132	LYS	3.3
18	R	25	THR	3.3
7	G	83	ALA	3.3
21	V	7	ARG	3.3
4	D	108	LEU	3.2
13	M	23	TYR	3.2
17	Q	25	ARG	3.2
16	P	30	GLY	3.2
13	M	12	ASN	3.2
4	D	135	LEU	3.2
12	L	98	TYR	3.2
17	Q	5	VAL	3.1
17	Q	9	VAL	3.1
2	B	186	ALA	3.1
17	Q	58	GLU	3.1
12	L	101	VAL	3.1
13	M	48	LEU	3.1
13	M	19	LEU	3.1
11	K	85	ARG	3.1
12	L	84	LEU	3.1
2	B	202	PRO	3.1
2	B	101	MET	3.1
18	R	29	PHE	3.1
4	D	125	HIS	3.0
20	T	77	ALA	3.0
19	S	49	ILE	3.0
20	T	103	GLY	3.0
4	D	45	GLN	3.0
13	M	31	LYS	3.0
17	Q	61	GLU	3.0
16	P	59	TRP	2.9
12	L	62	SER	2.9
1	A	1366	C	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	18	ARG	2.9
13	M	46	LYS	2.9
14	N	37	PHE	2.9
5	E	25	ARG	2.9
17	Q	101	ARG	2.9
11	K	21	ILE	2.8
18	R	84	LYS	2.8
17	Q	6	LEU	2.8
17	Q	59	ILE	2.8
10	J	59	SER	2.8
10	J	63	PHE	2.8
5	E	24	ARG	2.8
18	R	88	LYS	2.8
9	I	119	ALA	2.8
10	J	47	PHE	2.8
1	A	1443	G	2.8
17	Q	41	LYS	2.8
19	S	37	ARG	2.7
17	Q	2	PRO	2.7
13	M	24	GLY	2.7
19	S	38	SER	2.7
20	T	8	ARG	2.7
7	G	82	GLY	2.7
8	H	3	THR	2.7
17	Q	20	THR	2.7
16	P	29	ASP	2.7
4	D	126	ILE	2.7
20	T	72	LEU	2.7
2	B	31	TYR	2.7
6	F	63	TYR	2.7
12	L	86	ARG	2.7
16	P	34	GLU	2.6
16	P	53	VAL	2.6
2	B	135	GLN	2.6
6	F	97	PHE	2.6
19	S	40	ILE	2.6
7	G	101	LEU	2.6
20	T	17	ARG	2.6
10	J	55	LYS	2.6
12	L	56	ALA	2.6
2	B	187	LEU	2.5
13	M	41	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	228	GLY	2.5
5	E	31	LEU	2.5
21	V	21	TYR	2.5
13	M	15	VAL	2.5
19	S	12	ASP	2.5
16	P	6	LEU	2.5
12	L	102	ARG	2.5
17	Q	7	THR	2.5
17	Q	102	GLY	2.5
13	M	14	ARG	2.5
8	H	53	VAL	2.4
4	D	146	ILE	2.4
2	B	163	PHE	2.4
3	C	191	THR	2.4
18	R	24	ALA	2.4
10	J	74	ILE	2.4
17	Q	11	VAL	2.4
11	K	22	HIS	2.4
18	R	79	LEU	2.4
17	Q	68	ARG	2.3
2	B	133	LYS	2.3
5	E	120	THR	2.3
9	I	65	VAL	2.3
10	J	27	ALA	2.3
13	M	44	ARG	2.3
17	Q	70	ARG	2.3
1	A	972	C	2.3
20	T	26	ASN	2.3
21	V	5	ASP	2.3
16	P	18	ARG	2.3
10	J	54	PHE	2.3
2	B	201	ILE	2.3
5	E	119	LEU	2.2
13	M	102	ARG	2.2
17	Q	63	ARG	2.2
19	S	15	LEU	2.2
5	E	13	ILE	2.2
5	E	136	MET	2.2
17	Q	4	LYS	2.2
1	A	202	U	2.2
9	I	121	ARG	2.2
6	F	14	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
18	R	66	LEU	2.2
10	J	61	GLU	2.2
10	J	70	ARG	2.2
11	K	89	ALA	2.2
7	G	42	ILE	2.1
12	L	28	LYS	2.1
7	G	5	ARG	2.1
7	G	26	PHE	2.1
4	D	5	ILE	2.1
19	S	33	THR	2.1
3	C	157	ILE	2.1
5	E	76	ILE	2.1
5	E	101	ILE	2.1
12	L	67	THR	2.1
17	Q	88	TYR	2.1
20	T	56	MET	2.1
6	F	99	ALA	2.1
12	L	26	ALA	2.1
17	Q	92	ARG	2.1
14	N	39	LEU	2.1
17	Q	22	LEU	2.1
9	I	16	ARG	2.1
18	R	34	TYR	2.1
13	M	30	ALA	2.1
17	Q	21	VAL	2.1
11	K	43	SER	2.1
12	L	111	LYS	2.1
16	P	32	TYR	2.1
13	M	60	VAL	2.1
5	E	43	LEU	2.0
16	P	38	TYR	2.0
4	D	148	VAL	2.0
4	D	205	GLU	2.0
17	Q	57	VAL	2.0
17	Q	45	HIS	2.0
17	Q	74	LEU	2.0
20	T	19	SER	2.0
13	M	47	ASP	2.0
21	V	18	TYR	2.0
13	M	39	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1669	1/1	0.91	1.00	28.23	128,128,128,128	0
23	MG	A	1697	1/1	0.94	0.61	21.60	113,113,113,113	0
23	MG	A	1696	1/1	0.81	0.93	7.76	121,121,121,121	0
23	MG	A	1633	1/1	0.98	0.55	5.71	106,106,106,106	0
23	MG	A	1694	1/1	0.93	0.29	4.63	176,176,176,176	0
23	MG	A	1632	1/1	0.96	0.47	3.82	95,95,95,95	0
23	MG	A	1677	1/1	0.97	0.20	3.71	132,132,132,132	0
23	MG	A	1643	1/1	0.95	0.24	2.76	127,127,127,127	0
23	MG	A	1635	1/1	0.91	0.26	2.20	97,97,97,97	0
23	MG	A	1627	1/1	0.95	0.35	1.96	93,93,93,93	0
22	T1C	A	1601	42/42	0.94	0.20	1.65	173,207,227,233	0
23	MG	A	1700	1/1	0.97	0.16	1.64	137,137,137,137	0
23	MG	A	1658	1/1	0.90	0.26	1.64	120,120,120,120	0
24	ZN	D	301	1/1	0.99	0.39	1.44	175,175,175,175	0
23	MG	A	1685	1/1	0.98	0.19	0.85	109,109,109,109	0
23	MG	A	1624	1/1	0.93	0.20	0.57	122,122,122,122	0
23	MG	A	1665	1/1	0.96	0.19	0.33	101,101,101,101	0
23	MG	A	1682	1/1	0.94	0.19	0.22	109,109,109,109	0
24	ZN	N	101	1/1	0.99	0.23	-0.01	209,209,209,209	0
23	MG	A	1662	1/1	0.85	0.09	-0.48	138,138,138,138	0
23	MG	A	1690	1/1	0.95	0.17	-0.59	114,114,114,114	0
23	MG	A	1611	1/1	0.97	0.11	-0.74	131,131,131,131	0
23	MG	A	1618	1/1	0.96	0.10	-	120,120,120,120	0
23	MG	A	1687	1/1	0.83	0.20	-	145,145,145,145	0
23	MG	A	1640	1/1	0.96	0.34	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1686	1/1	0.78	0.15	-	146,146,146,146	0
23	MG	A	1666	1/1	0.97	0.41	-	89,89,89,89	0
23	MG	A	1620	1/1	0.96	0.14	-	106,106,106,106	0
23	MG	A	1699	1/1	0.99	0.18	-	121,121,121,121	0
23	MG	A	1639	1/1	0.96	0.13	-	132,132,132,132	0
23	MG	A	1688	1/1	0.99	0.18	-	140,140,140,140	0
23	MG	A	1679	1/1	0.95	0.18	-	130,130,130,130	0
23	MG	A	1702	1/1	0.99	0.12	-	127,127,127,127	0
23	MG	A	1672	1/1	0.98	0.41	-	111,111,111,111	0
23	MG	A	1654	1/1	0.78	1.38	-	117,117,117,117	0
23	MG	A	1644	1/1	0.94	0.18	-	132,132,132,132	0
23	MG	A	1622	1/1	0.84	0.87	-	133,133,133,133	0
23	MG	A	1623	1/1	0.82	0.50	-	113,113,113,113	0
23	MG	A	1674	1/1	0.92	0.21	-	125,125,125,125	0
23	MG	A	1671	1/1	0.96	0.22	-	120,120,120,120	0
23	MG	E	201	1/1	0.91	0.18	-	109,109,109,109	0
23	MG	A	1675	1/1	0.97	0.31	-	135,135,135,135	0
23	MG	A	1606	1/1	0.84	0.71	-	117,117,117,117	0
23	MG	A	1629	1/1	0.97	0.56	-	113,113,113,113	0
23	MG	A	1636	1/1	0.81	0.52	-	105,105,105,105	0
23	MG	A	1695	1/1	0.74	0.56	-	124,124,124,124	0
23	MG	A	1610	1/1	0.83	0.30	-	144,144,144,144	0
23	MG	A	1619	1/1	0.60	0.55	-	143,143,143,143	0
23	MG	A	1667	1/1	0.98	0.20	-	111,111,111,111	0
23	MG	A	1613	1/1	0.83	0.37	-	136,136,136,136	0
23	MG	A	1646	1/1	0.89	0.80	-	122,122,122,122	0
23	MG	A	1678	1/1	0.93	0.55	-	117,117,117,117	0
23	MG	A	1655	1/1	0.90	0.25	-	112,112,112,112	0
23	MG	A	1641	1/1	0.95	0.30	-	98,98,98,98	0
23	MG	A	1612	1/1	0.81	0.48	-	117,117,117,117	0
23	MG	A	1693	1/1	0.83	0.17	-	128,128,128,128	0
23	MG	A	1609	1/1	0.93	0.08	-	151,151,151,151	0
23	MG	A	1614	1/1	0.97	0.11	-	108,108,108,108	0
23	MG	A	1625	1/1	0.85	0.64	-	109,109,109,109	0
23	MG	A	1621	1/1	0.90	0.32	-	126,126,126,126	0
23	MG	A	1607	1/1	0.84	0.78	-	98,98,98,98	0
23	MG	A	1698	1/1	0.93	0.41	-	95,95,95,95	0
23	MG	A	1651	1/1	0.97	0.43	-	115,115,115,115	0
23	MG	A	1701	1/1	0.77	0.38	-	124,124,124,124	0
23	MG	A	1691	1/1	0.95	0.27	-	121,121,121,121	0
23	MG	A	1645	1/1	0.95	0.29	-	173,173,173,173	0
23	MG	A	1615	1/1	0.95	0.32	-	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1656	1/1	0.97	0.22	-	104,104,104,104	0
23	MG	A	1604	1/1	0.87	0.12	-	120,120,120,120	0
23	MG	A	1642	1/1	0.92	0.82	-	114,114,114,114	0
23	MG	A	1649	1/1	0.88	0.30	-	159,159,159,159	0
23	MG	A	1634	1/1	0.90	0.84	-	104,104,104,104	0
23	MG	A	1683	1/1	0.97	0.09	-	115,115,115,115	0
23	MG	A	1680	1/1	0.91	0.19	-	99,99,99,99	0
23	MG	A	1681	1/1	0.92	0.20	-	131,131,131,131	0
23	MG	A	1630	1/1	0.96	0.42	-	127,127,127,127	0
23	MG	A	1602	1/1	0.93	0.38	-	99,99,99,99	0
23	MG	A	1637	1/1	0.93	0.23	-	105,105,105,105	0
23	MG	A	1689	1/1	0.92	0.52	-	118,118,118,118	0
23	MG	A	1703	1/1	-	-	-	116,116,116,116	0
23	MG	A	1692	1/1	0.94	0.24	-	172,172,172,172	0
23	MG	A	1673	1/1	0.91	0.36	-	129,129,129,129	0
23	MG	A	1652	1/1	0.90	0.49	-	145,145,145,145	0
23	MG	A	1648	1/1	0.85	0.34	-	152,152,152,152	0
23	MG	A	1605	1/1	0.97	0.62	-	135,135,135,135	0
23	MG	A	1617	1/1	0.77	0.26	-	130,130,130,130	0
23	MG	A	1647	1/1	0.73	0.31	-	109,109,109,109	0
23	MG	A	1676	1/1	0.95	0.75	-	136,136,136,136	0
23	MG	A	1608	1/1	0.80	0.48	-	128,128,128,128	0
23	MG	A	1657	1/1	0.85	0.25	-	112,112,112,112	0
23	MG	A	1638	1/1	0.99	0.28	-	93,93,93,93	0
23	MG	A	1670	1/1	0.97	0.68	-	123,123,123,123	0
23	MG	A	1653	1/1	0.90	0.81	-	114,114,114,114	0
23	MG	A	1660	1/1	0.93	0.11	-	141,141,141,141	0
23	MG	A	1650	1/1	0.84	0.10	-	131,131,131,131	0
23	MG	A	1616	1/1	0.83	0.07	-	125,125,125,125	0
23	MG	A	1684	1/1	0.95	0.30	-	138,138,138,138	0
23	MG	A	1603	1/1	0.88	0.44	-	127,127,127,127	0
23	MG	A	1626	1/1	0.80	0.50	-	125,125,125,125	0
23	MG	A	1661	1/1	0.98	0.54	-	119,119,119,119	0
23	MG	A	1664	1/1	0.40	0.86	-	136,136,136,136	0
23	MG	A	1631	1/1	0.95	0.09	-	118,118,118,118	0
23	MG	A	1668	1/1	0.89	0.74	-	123,123,123,123	0
23	MG	A	1659	1/1	0.97	0.33	-	106,106,106,106	0
23	MG	A	1628	1/1	0.98	0.21	-	139,139,139,139	0
23	MG	A	1663	1/1	0.90	0.25	-	97,97,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.