



# Full wwPDB X-ray Structure Validation Report i

Mar 31, 2014 – 05:44 PM BST

PDB ID : 3V2C  
Title : Crystal structure of YfiA bound to the 70S ribosome. This PDB entry contains coordinates for the 30S subunit with bound YfiA of the 1st ribosome in the ASU  
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.  
Deposited on : 2011-12-12  
Resolution : 2.70 Å(reported)

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

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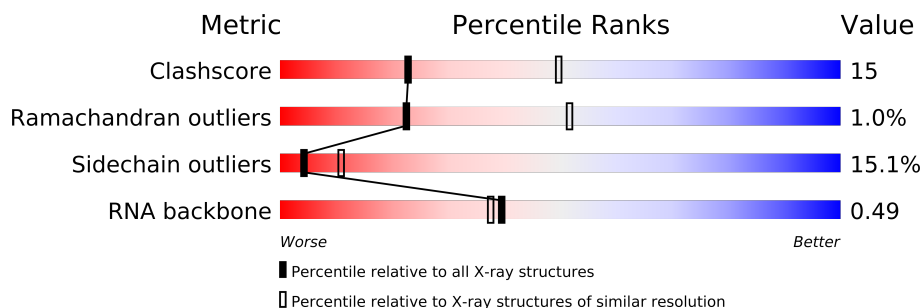
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	<b>NOT EXECUTED</b>
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23004

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RNA backbone	1838	1042 (3.20-2.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	

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Mol	Chain	Length	Quality of chain
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	Y	119	

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 51116 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1493	Total	C	N	O	P	0	0	0
			32102	14287	5955	10367	1493			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1777	1134	318	320	5			

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1520	960	283	272	5			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			781	495	137	146	3			

- 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
			1167	727	224	210	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
			1045	665	188	190	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	125	Total	C	N	O	0	0	0
			852	533	163	156			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	96	Total	C	N	O	0	0	0
			659	408	131	120			

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	122	Total	C	N	O	S	0	0	0
			909	570	179	159	1			

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	114	Total	C	N	O	S	0	0	0
			801	494	164	142	1			

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			478	303	99	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
			724	453	143	126	2			

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	68	Total	C	N	O	0	0	0
			514	329	98	87			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	96	Total	C	N	O	S	0	0	0
			699	430	150	117	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	95	Total	C	N	O	S	0	0	0
			754	472	142	137	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	114	HIS	-	EXPRESSION TAG	UNP P0AD49
Y	115	HIS	-	EXPRESSION TAG	UNP P0AD49
Y	116	HIS	-	EXPRESSION TAG	UNP P0AD49
Y	117	HIS	-	EXPRESSION TAG	UNP P0AD49
Y	118	HIS	-	EXPRESSION TAG	UNP P0AD49
Y	119	HIS	-	EXPRESSION TAG	UNP P0AD49

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	P	1	Total	Mg	0	0
			1	1		
23	D	2	Total	Mg	0	0
			2	2		
23	E	1	Total	Mg	0	0
			1	1		
23	I	1	Total	Mg	0	0
			1	1		
23	A	223	Total	Mg	0	0
			223	223		
23	O	1	Total	Mg	0	0
			1	1		
23	L	1	Total	Mg	0	0
			1	1		
23	F	1	Total	Mg	0	0
			1	1		
23	M	2	Total	Mg	0	0
			2	2		

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

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	460	Total 460	O 460	0	0
25	D	3	Total 3	O 3	0	0
25	E	2	Total 2	O 2	0	0
25	F	2	Total 2	O 2	0	0
25	G	2	Total 2	O 2	0	0
25	J	1	Total 1	O 1	0	0
25	K	1	Total 1	O 1	0	0
25	L	3	Total 3	O 3	0	0
25	M	1	Total 1	O 1	0	0
25	O	4	Total 4	O 4	0	0
25	Q	3	Total 3	O 3	0	0
25	Y	1	Total 1	O 1	0	0

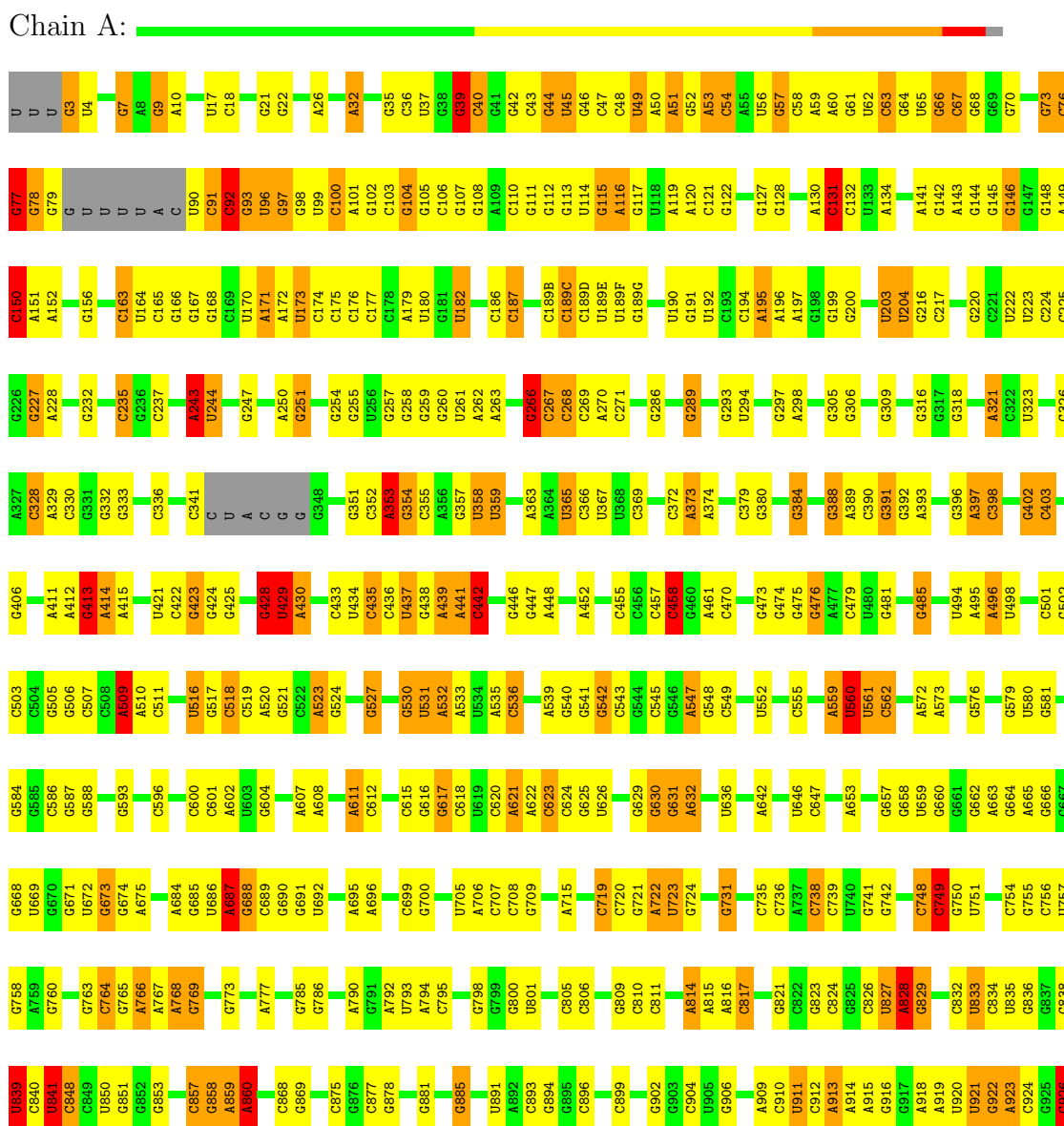


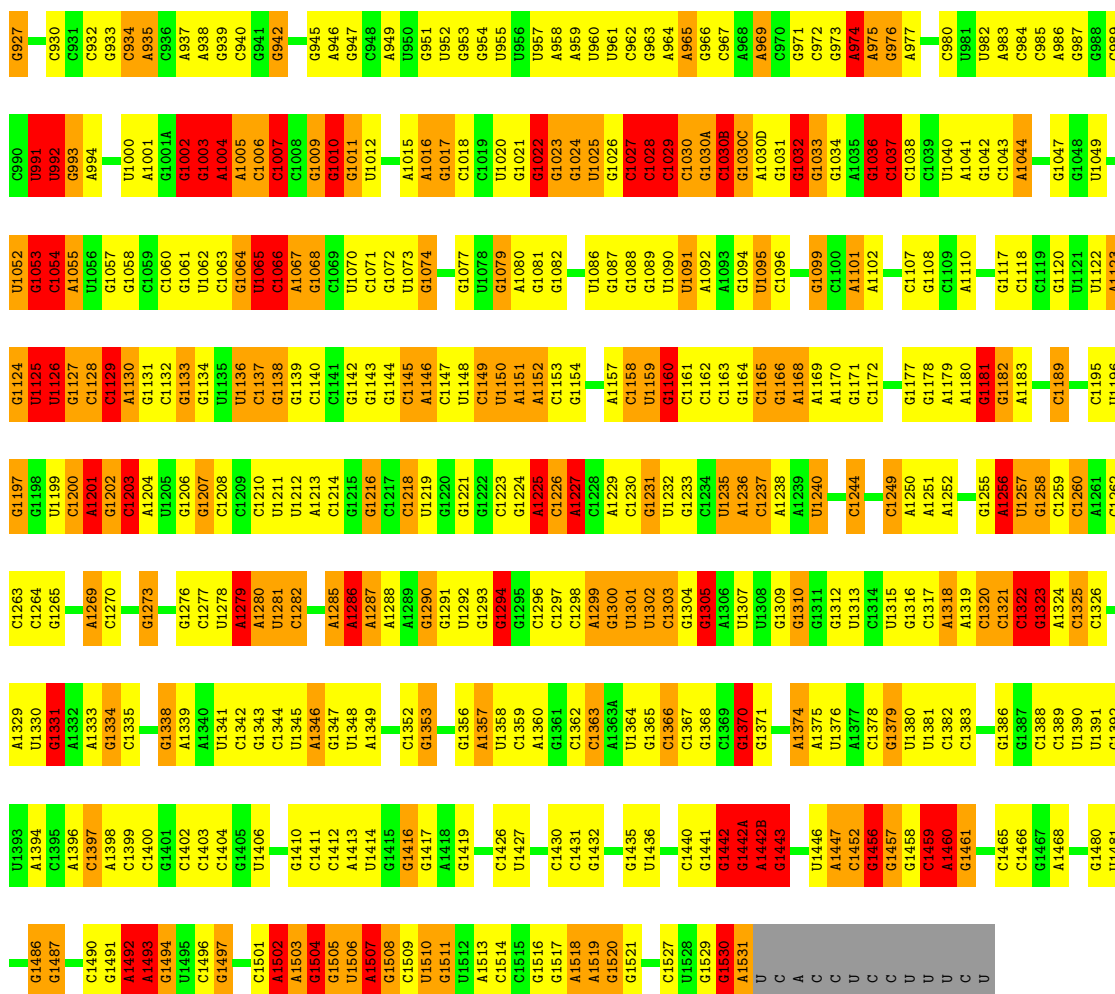
### 3 Residue-property plots

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

Note EDS was not executed.

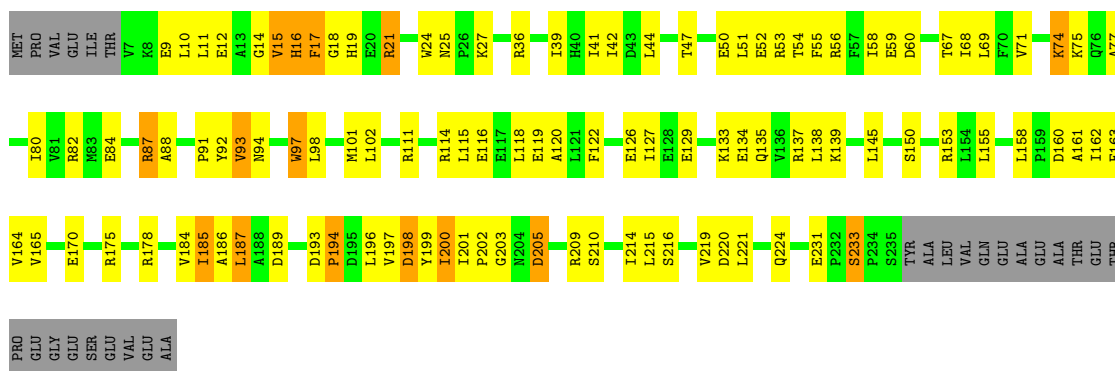
- Molecule 1: 16S Ribosomal RNA





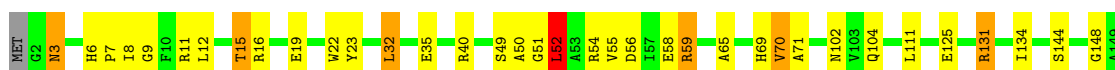
- Molecule 2: 30S Ribosomal Protein S2

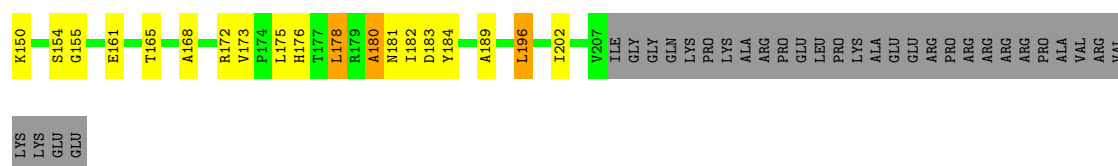
Chain B:



- Molecule 3: 30S Ribosomal Protein S3

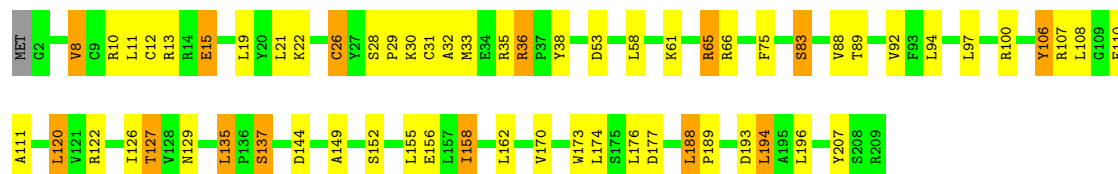
Chain C:





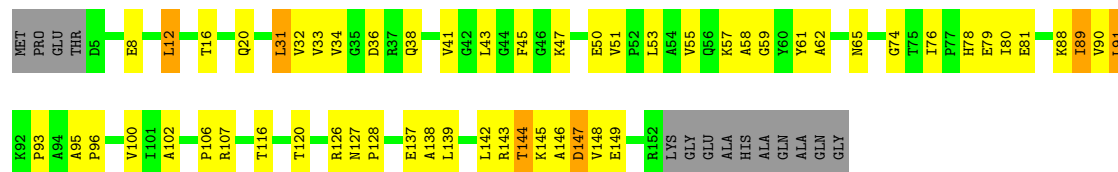
• Molecule 4: 30S Ribosomal Protein S4

Chain D:



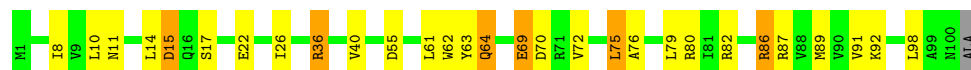
• Molecule 5: 30S Ribosomal Protein S5

Chain E:



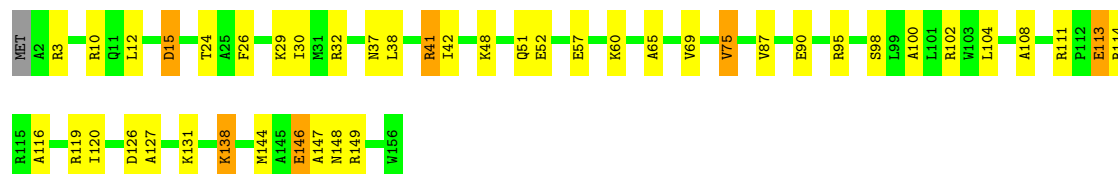
• Molecule 6: 30S Ribosomal Protein S6

Chain F:



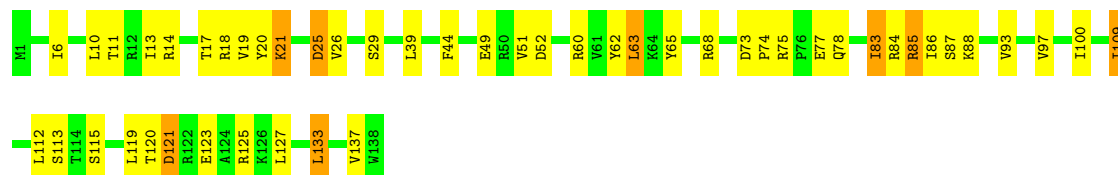
• Molecule 7: 30S Ribosomal Protein S7

Chain G:



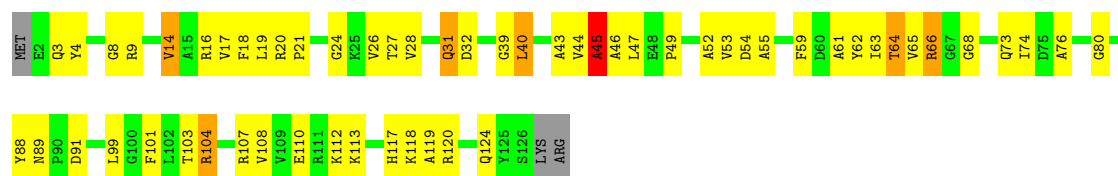
• Molecule 8: 30S Ribosomal Protein S8

Chain H:



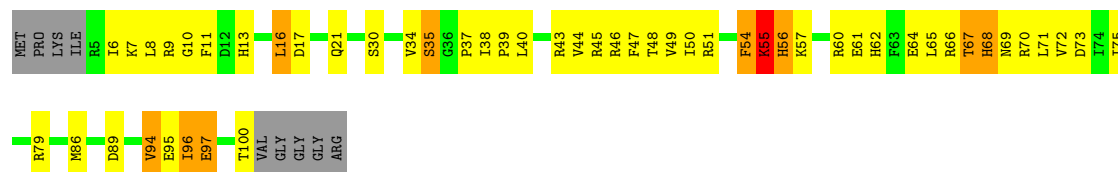
• Molecule 9: 30S Ribosomal Protein S9

Chain I: 



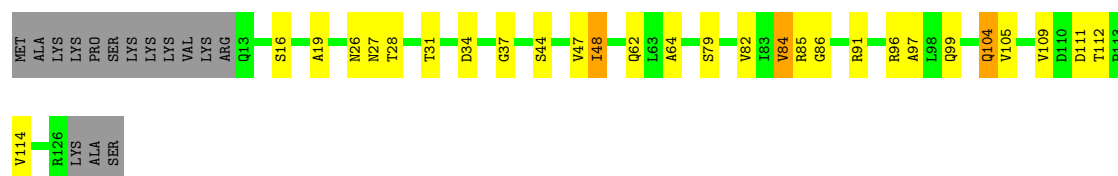
- Molecule 10: 30S Ribosomal Protein S10

Chain J: 



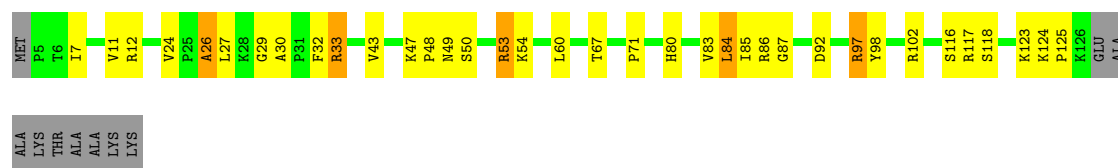
- Molecule 11: 30S Ribosomal Protein S11

Chain K: 



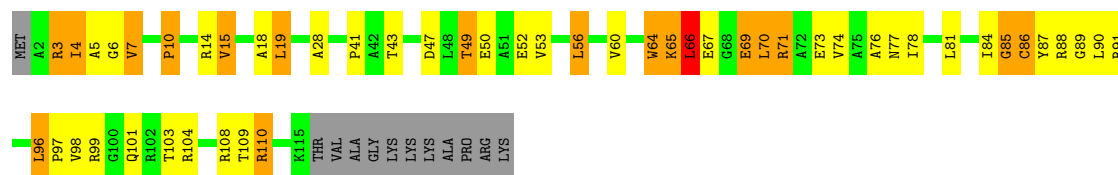
- Molecule 12: 30S Ribosomal Protein S12

Chain L: 



- Molecule 13: 30S Ribosomal Protein S13

Chain M: 



- Molecule 14: 30S Ribosomal Protein S14

Chain N: 



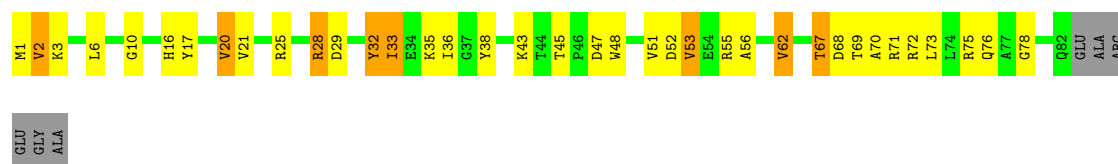
- Molecule 15: 30S Ribosomal Protein S15

Chain O:



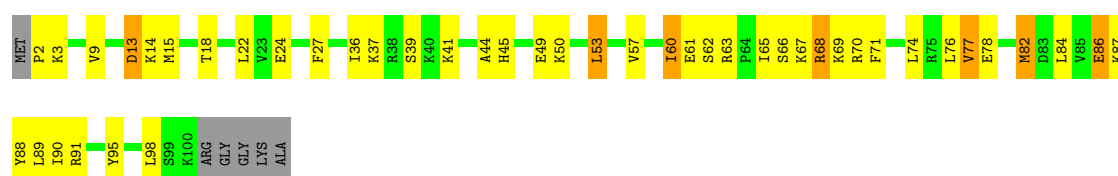
- Molecule 16: 30S Ribosomal Protein S16

Chain P:



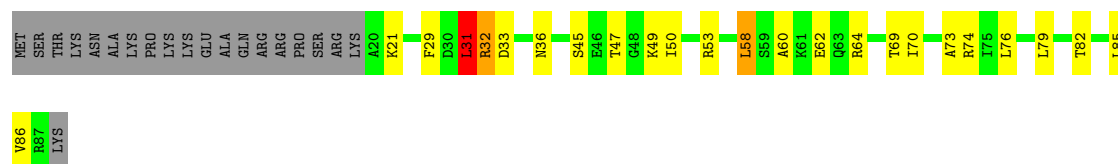
- Molecule 17: 30S Ribosomal Protein S17

Chain Q:



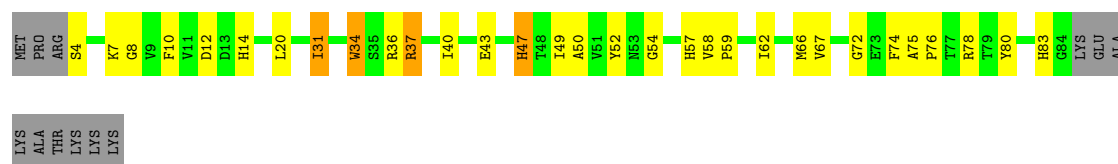
- Molecule 18: 30S Ribosomal Protein S18

Chain R:



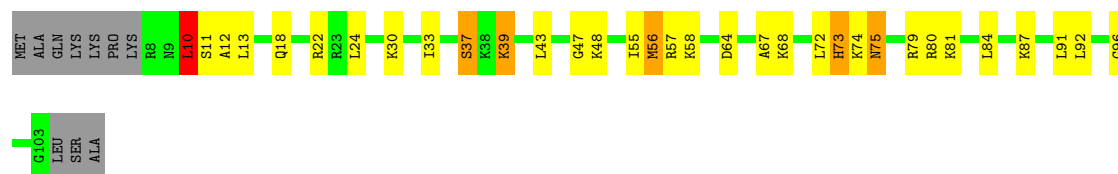
- Molecule 19: 30S Ribosomal Protein S19

Chain S:



- Molecule 20: 30S Ribosomal Protein S20

Chain T:



- Molecule 21: 30S Ribosomal Protein THX

Chain U:



- Molecule 22: Ribosome-associated inhibitor A

Chain Y: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.63Å 449.30Å 620.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.71 – 2.70	Depositor
% Data completeness (in resolution range)	98.4 (49.71-2.70)	Depositor
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2.869)	Depositor
R, $R_{free}$	0.217 , 0.254	Depositor
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.155	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 1557851 reflections	Xtriage
Total number of atoms	51116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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

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	1.00	41/35935 (0.1%)	1.48	589/56084 (1.1%)
2	B	0.57	0/1811	0.74	0/2452
3	C	0.63	1/1474 (0.1%)	0.84	1/2003 (0.0%)
4	D	0.73	2/1550 (0.1%)	0.87	1/2106 (0.0%)
5	E	0.60	0/1121	0.78	0/1517
6	F	0.61	0/794	0.79	0/1082
7	G	0.59	0/1186	0.74	0/1603
8	H	0.52	0/1065	0.71	0/1445
9	I	0.60	0/867	0.85	0/1180
10	J	0.65	0/672	0.83	0/919
11	K	0.59	0/843	0.74	0/1144
12	L	0.67	0/925	0.83	0/1251
13	M	0.66	0/811	0.91	0/1103
14	N	0.62	0/487	0.83	0/649
15	O	0.59	0/735	0.84	2/981 (0.2%)
16	P	0.60	0/667	0.83	0/905
17	Q	0.59	0/836	0.76	0/1117
18	R	0.51	0/519	0.82	1/699 (0.1%)
19	S	0.58	0/574	0.85	1/781 (0.1%)
20	T	0.59	0/701	0.86	2/930 (0.2%)
21	U	0.57	0/203	0.73	0/266
22	Y	0.67	0/766	0.87	0/1034
All	All	0.89	44/54542 (0.1%)	1.31	597/81251 (0.7%)

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
2	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
4	D	0	1
9	I	0	3
10	J	0	3
13	M	0	2
18	R	0	1
All	All	0	13

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1459	C	N1-C2	18.78	1.58	1.40
1	A	1442(A)	G	N9-C4	13.88	1.49	1.38
1	A	1459	C	C1'-N1	11.90	1.66	1.48
1	A	1442(A)	G	C2-N3	11.18	1.41	1.32
1	A	1459	C	C2-N3	11.00	1.44	1.35
4	D	12	CYS	CB-SG	10.70	2.00	1.82
1	A	52	G	P-OP2	-10.33	1.31	1.49
1	A	66	G	P-OP1	-10.09	1.31	1.49
1	A	187	C	P-OP2	-9.49	1.32	1.49
1	A	341	C	P-OP1	-9.44	1.32	1.49
1	A	615	C	P-OP2	-9.07	1.33	1.49
1	A	542	G	P-OP1	-8.90	1.33	1.49
1	A	516	U	P-OP2	-8.76	1.34	1.49
1	A	516	U	P-OP1	-8.73	1.34	1.49
1	A	1442(A)	G	P-OP1	-8.72	1.34	1.49
4	D	26	CYS	CB-SG	8.66	1.97	1.82
1	A	341	C	P-OP2	-8.56	1.34	1.49
1	A	1227	A	N9-C4	-8.53	1.32	1.37
1	A	542	G	P-OP2	-8.49	1.34	1.49
1	A	615	C	P-OP1	-8.39	1.34	1.49
1	A	1442(A)	G	C5-C6	8.38	1.50	1.42
1	A	1442(A)	G	P-OP2	-8.35	1.34	1.49
1	A	1442(A)	G	N3-C4	8.26	1.41	1.35
1	A	439	A	P-OP2	-8.13	1.35	1.49
1	A	44	G	P-OP2	-7.87	1.35	1.49
1	A	44	G	P-OP1	-7.79	1.35	1.49
1	A	187	C	P-OP1	-7.65	1.35	1.49
1	A	439	A	P-OP1	-7.48	1.36	1.49
1	A	1442(A)	G	C6-N1	6.99	1.44	1.39
1	A	1443	G	C6-O6	-6.34	1.18	1.24
1	A	965	A	N9-C4	-5.78	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1519	A	N7-C5	-5.72	1.35	1.39
1	A	1125	U	P-O5'	5.57	1.65	1.59
1	A	1502	A	N9-C4	-5.57	1.34	1.37
1	A	1459	C	C2-O2	5.54	1.29	1.24
1	A	1493	A	N9-C4	5.53	1.41	1.37
1	A	1201	A	N3-C4	5.40	1.38	1.34
3	C	56	ASP	CB-CG	5.33	1.62	1.51
1	A	358	U	N3-C4	-5.22	1.33	1.38
1	A	53	A	C6-N1	-5.21	1.31	1.35
1	A	398	C	C4-C5	5.18	1.47	1.43
1	A	1125	U	O3'-P	5.10	1.67	1.61
1	A	1492	A	N9-C4	5.07	1.40	1.37
1	A	1256	A	N9-C4	5.00	1.40	1.37

All (597) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1459	C	C6-N1-C2	-31.41	107.74	120.30
1	A	1459	C	N3-C2-O2	-28.10	102.23	121.90
1	A	1442(A)	G	N3-C4-C5	-24.94	116.13	128.60
1	A	1459	C	N1-C2-O2	19.91	130.84	118.90
1	A	1442(A)	G	C6-N1-C2	-19.29	113.52	125.10
1	A	1442(A)	G	C2-N3-C4	18.67	121.24	111.90
1	A	1442(B)	A	N1-C2-N3	18.55	138.57	129.30
1	A	1442(A)	G	N3-C4-N9	17.90	136.74	126.00
1	A	1442(A)	G	C5-C6-N1	17.75	120.38	111.50
1	A	1459	C	C2-N1-C1'	17.11	137.62	118.80
1	A	53	A	C6-N1-C2	13.45	126.67	118.60
1	A	365	U	C5-C6-N1	-12.96	116.22	122.70
1	A	1442(A)	G	C8-N9-C4	-12.38	101.45	106.40
1	A	358	U	C2-N3-C4	12.36	134.42	127.00
1	A	1459	C	C2-N3-C4	-12.27	113.77	119.90
1	A	1442(A)	G	C4-N9-C1'	11.76	141.79	126.50
1	A	39	G	C5-C6-O6	-11.37	121.78	128.60
1	A	1459	C	C5-C6-N1	11.07	126.53	121.00
1	A	1459	C	N1-C2-N3	11.04	126.93	119.20
1	A	1123	A	C6-N1-C2	10.90	125.14	118.60
1	A	40	C	C6-N1-C2	10.89	124.66	120.30
1	A	1502	A	C2-N3-C4	-10.85	105.18	110.60
1	A	1150	U	C2-N3-C4	10.80	133.48	127.00
1	A	403	C	N3-C4-C5	-10.50	117.70	121.90
1	A	1460	A	C5-N7-C8	10.44	109.12	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	C	C2-N3-C4	-10.18	114.81	119.90
1	A	1150	U	N3-C4-C5	-10.15	108.51	114.60
1	A	1227	A	C2-N3-C4	-10.00	105.60	110.60
1	A	992	U	N3-C2-O2	-9.97	115.22	122.20
1	A	1126	U	C5-C6-N1	9.78	127.59	122.70
1	A	1126	U	C2-N1-C1'	9.75	129.40	117.70
4	D	12	CYS	CA-CB-SG	9.69	131.44	114.00
1	A	1335	C	C6-N1-C2	9.64	124.16	120.30
1	A	1460	A	N1-C6-N6	-9.54	112.88	118.60
1	A	1502	A	C5-N7-C8	-9.48	99.16	103.90
1	A	39	G	N1-C2-N3	-9.48	118.21	123.90
1	A	357	G	C6-N1-C2	9.32	130.69	125.10
1	A	1502	A	N1-C2-N3	9.31	133.95	129.30
1	A	1443	G	C5-C6-N1	9.31	116.15	111.50
1	A	1502	A	N7-C8-N9	9.30	118.45	113.80
1	A	398	C	N3-C4-C5	9.28	125.61	121.90
1	A	1442(B)	A	C2-N3-C4	-9.26	105.97	110.60
1	A	839	U	N1-C2-O2	9.25	129.28	122.80
1	A	54	C	C2-N3-C4	9.22	124.51	119.90
1	A	39	G	N1-C6-O6	9.03	125.31	119.90
1	A	1460	A	N7-C8-N9	-8.96	109.32	113.80
1	A	1181	G	C4-N9-C1'	-8.93	114.90	126.50
1	A	1442(A)	G	N1-C2-N2	-8.93	108.17	116.20
1	A	44	G	N1-C6-O6	-8.66	114.70	119.90
1	A	1027	C	C5-C4-N4	8.66	126.26	120.20
1	A	53	A	C5-C6-N1	-8.60	113.40	117.70
1	A	396	G	C5-C6-O6	8.47	133.68	128.60
1	A	1058	G	N9-C4-C5	-8.39	102.04	105.40
1	A	398	C	N3-C4-N4	-8.34	112.16	118.00
1	A	896	C	C6-N1-C2	8.33	123.63	120.30
1	A	402	G	N1-C6-O6	8.32	124.89	119.90
1	A	402	G	C5-C6-N1	-8.29	107.36	111.50
1	A	1459	C	C4-C5-C6	8.22	121.51	117.40
1	A	1024	G	N7-C8-N9	8.20	117.20	113.10
1	A	403	C	N1-C2-O2	-8.19	113.98	118.90
1	A	1443	G	N1-C6-O6	-8.19	114.98	119.90
1	A	1442(A)	G	C8-N9-C1'	-8.16	116.39	127.00
1	A	40	C	N3-C2-O2	8.15	127.61	121.90
1	A	365	U	C2-N1-C1'	-8.14	107.93	117.70
1	A	1123	A	C5-C6-N6	8.11	130.19	123.70
1	A	1197	G	N3-C4-C5	-8.07	124.57	128.60
1	A	1442(A)	G	N1-C6-O6	-8.06	115.07	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	913	A	C8-N9-C4	-8.04	102.58	105.80
1	A	396	G	N1-C6-O6	-8.03	115.08	119.90
1	A	1197	G	N3-C4-N9	8.02	130.81	126.00
1	A	1027	C	N3-C4-N4	-8.00	112.40	118.00
1	A	992	U	N1-C2-O2	8.00	128.40	122.80
1	A	1099	G	C8-N9-C4	-7.99	103.21	106.40
1	A	365	U	C4-C5-C6	7.98	124.49	119.70
1	A	1126	U	C5-C4-O4	-7.97	121.12	125.90
1	A	357	G	N1-C2-N2	7.94	123.34	116.20
1	A	1504	G	C8-N9-C4	7.93	109.57	106.40
1	A	1150	U	C5-C4-O4	7.93	130.66	125.90
1	A	1054	C	N3-C4-C5	7.92	125.07	121.90
1	A	45	U	C2-N3-C4	-7.86	122.28	127.00
1	A	1460	A	C4-C5-N7	-7.83	106.78	110.70
1	A	1527	C	C6-N1-C2	7.80	123.42	120.30
1	A	1363	C	C6-N1-C2	-7.74	117.21	120.30
1	A	1227	A	N3-C4-C5	7.73	132.21	126.80
1	A	523	A	C5-N7-C8	-7.73	100.03	103.90
1	A	403	C	C2-N3-C4	7.69	123.74	119.90
1	A	1442(A)	G	N3-C2-N2	7.65	125.25	119.90
1	A	1443	G	C4-C5-C6	-7.65	114.21	118.80
1	A	1507	A	N1-C6-N6	7.64	123.18	118.60
1	A	1030	C	N1-C2-O2	7.57	123.44	118.90
1	A	53	A	N1-C2-N3	-7.56	125.52	129.30
1	A	974	A	C8-N9-C4	-7.54	102.78	105.80
1	A	40	C	N1-C2-N3	-7.51	113.94	119.20
1	A	1181	G	C8-N9-C1'	7.51	136.76	127.00
1	A	1058	G	C5-C6-O6	-7.50	124.10	128.60
1	A	795	C	C6-N1-C2	-7.50	117.30	120.30
1	A	1468	A	C5-C6-N6	-7.50	117.70	123.70
1	A	1029	C	N3-C2-O2	-7.48	116.67	121.90
1	A	1003	G	N1-C6-O6	-7.47	115.42	119.90
1	A	39	G	N1-C2-N2	7.47	122.92	116.20
1	A	1037	C	N3-C4-C5	-7.44	118.93	121.90
1	A	403	C	C6-N1-C2	-7.42	117.33	120.30
20	T	10	LEU	CA-CB-CG	7.41	132.34	115.30
1	A	366	C	C6-N1-C2	7.37	123.25	120.30
1	A	839	U	N3-C2-O2	-7.32	117.07	122.20
1	A	1058	G	C8-N9-C4	7.31	109.32	106.40
1	A	1029	C	N3-C4-N4	-7.30	112.89	118.00
1	A	1024	G	C8-N9-C4	-7.29	103.48	106.40
1	A	54	C	N3-C4-C5	-7.26	118.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1159	U	C5-C4-O4	7.25	130.25	125.90
1	A	1357	A	N7-C8-N9	7.25	117.42	113.80
1	A	355	C	C6-N1-C2	-7.23	117.41	120.30
1	A	1520	G	C8-N9-C4	7.23	109.29	106.40
1	A	992	U	C6-N1-C2	-7.21	116.67	121.00
1	A	1357	A	C8-N9-C4	-7.21	102.92	105.80
1	A	1442	G	C5-N7-C8	7.21	107.90	104.30
1	A	1003	G	N9-C4-C5	7.18	108.27	105.40
1	A	858	G	C8-N9-C4	-7.17	103.53	106.40
1	A	1224	G	C4-C5-N7	-7.16	107.94	110.80
1	A	1504	G	C4-N9-C1'	-7.16	117.19	126.50
1	A	1518	A	C5-C6-N6	7.15	129.42	123.70
1	A	1091	U	N3-C2-O2	-7.14	117.20	122.20
1	A	1530	G	N1-C6-O6	7.12	124.17	119.90
1	A	1066	C	N1-C2-O2	7.10	123.16	118.90
1	A	1518	A	N9-C4-C5	7.10	108.64	105.80
1	A	39	G	C4-C5-C6	-7.10	114.54	118.80
1	A	40	C	C2-N1-C1'	-7.10	110.99	118.80
1	A	150	C	C5-C6-N1	7.08	124.54	121.00
1	A	523	A	N7-C8-N9	7.08	117.34	113.80
1	A	754	C	N1-C2-O2	7.06	123.14	118.90
1	A	1502	A	C6-C5-N7	-7.06	127.36	132.30
1	A	359	U	N1-C2-O2	-7.05	117.86	122.80
1	A	1281	U	C5-C6-N1	7.04	126.22	122.70
1	A	754	C	N3-C2-O2	-7.04	116.97	121.90
1	A	52	G	C5-C6-N1	-7.03	107.99	111.50
1	A	92	C	N3-C4-N4	6.99	122.89	118.00
1	A	1397	C	C2-N1-C1'	6.99	126.49	118.80
1	A	839	U	C2-N1-C1'	6.98	126.08	117.70
1	A	695	A	C8-N9-C4	-6.97	103.01	105.80
1	A	40	C	C4-C5-C6	-6.95	113.93	117.40
1	A	227	G	C8-N9-C4	6.95	109.18	106.40
1	A	1181	G	N3-C4-C5	6.94	132.07	128.60
1	A	560	U	C5-C6-N1	6.93	126.17	122.70
1	A	1442(A)	G	N7-C8-N9	6.92	116.56	113.10
1	A	521	G	N1-C6-O6	-6.90	115.76	119.90
1	A	402	G	C6-C5-N7	-6.90	126.26	130.40
1	A	1227	A	N3-C4-N9	-6.90	121.88	127.40
1	A	579	G	C8-N9-C4	-6.89	103.65	106.40
1	A	1123	A	N3-C4-N9	-6.89	121.89	127.40
1	A	1158	C	C4-C5-C6	6.88	120.84	117.40
1	A	1386	G	C2-N3-C4	6.88	115.34	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	A	C8-N9-C4	-6.87	103.05	105.80
1	A	54	C	N1-C2-O2	-6.87	114.78	118.90
1	A	77	G	N9-C4-C5	-6.86	102.66	105.40
1	A	1129	C	C6-N1-C2	-6.85	117.56	120.30
1	A	1074	G	N1-C6-O6	6.85	124.01	119.90
1	A	1154	G	C8-N9-C4	6.85	109.14	106.40
1	A	40	C	C5-C4-N4	-6.81	115.44	120.20
1	A	1286	A	C8-N9-C4	-6.81	103.08	105.80
1	A	1054	C	C2-N3-C4	-6.80	116.50	119.90
1	A	365	U	C2-N3-C4	-6.80	122.92	127.00
1	A	1442(A)	G	C5-C6-O6	-6.79	124.53	128.60
1	A	44	G	C5-C6-O6	6.76	132.66	128.60
1	A	403	C	N3-C2-O2	6.76	126.63	121.90
1	A	1442(B)	A	C6-N1-C2	-6.76	114.54	118.60
1	A	326	G	C5-C6-O6	6.76	132.65	128.60
1	A	1290	G	C8-N9-C4	-6.75	103.70	106.40
1	A	1460	A	C6-C5-N7	6.75	137.03	132.30
1	A	1197	G	C4-N9-C1'	6.75	135.28	126.50
1	A	1493	A	C8-N9-C4	-6.75	103.10	105.80
1	A	913	A	N9-C4-C5	6.72	108.49	105.80
1	A	1519	A	C8-N9-C4	-6.72	103.11	105.80
1	A	621	A	N1-C6-N6	-6.70	114.58	118.60
1	A	560	U	C2-N1-C1'	6.69	125.72	117.70
1	A	927	G	C8-N9-C4	6.68	109.07	106.40
1	A	1518	A	C4-C5-N7	-6.68	107.36	110.70
1	A	54	C	N3-C2-O2	6.68	126.58	121.90
1	A	47	C	N3-C4-N4	-6.67	113.33	118.00
1	A	297	G	C8-N9-C4	6.67	109.07	106.40
1	A	893	C	N3-C4-C5	6.67	124.57	121.90
1	A	1456	G	C4-N9-C1'	-6.67	117.83	126.50
1	A	899	C	C6-N1-C2	6.66	122.97	120.30
1	A	318	G	N3-C2-N2	-6.63	115.26	119.90
1	A	1276	G	C8-N9-C4	-6.62	103.75	106.40
1	A	814	A	C8-N9-C4	6.62	108.45	105.80
1	A	357	G	N3-C4-C5	6.62	131.91	128.60
1	A	187	C	N1-C2-O2	6.61	122.87	118.90
1	A	402	G	C2-N3-C4	-6.61	108.60	111.90
1	A	1099	G	N9-C4-C5	6.60	108.04	105.40
1	A	836	G	N1-C6-O6	6.60	123.86	119.90
1	A	1519	A	C5-C6-N1	-6.58	114.41	117.70
1	A	893	C	N1-C2-O2	6.57	122.84	118.90
1	A	396	G	C4-C5-N7	-6.56	108.17	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	52	LEU	CA-CB-CG	6.54	130.34	115.30
1	A	44	G	C6-N1-C2	-6.53	121.18	125.10
1	A	1030	C	C2-N3-C4	6.53	123.16	119.90
1	A	1430	C	N3-C4-C5	6.53	124.51	121.90
1	A	1530	G	C5-C6-O6	-6.52	124.69	128.60
1	A	1502	A	C8-N9-C4	-6.52	103.19	105.80
1	A	1123	A	C5-C6-N1	-6.51	114.44	117.70
1	A	1022	G	N3-C2-N2	6.50	124.45	119.90
1	A	1149	C	N1-C2-O2	6.50	122.80	118.90
1	A	44	G	N1-C2-N3	6.50	127.80	123.90
1	A	1290	G	N3-C4-C5	-6.48	125.36	128.60
19	S	8	GLY	N-CA-C	-6.47	96.92	113.10
1	A	1126	U	C6-N1-C1'	-6.46	112.15	121.20
1	A	1460	A	C5-C6-N6	6.46	128.87	123.70
1	A	1037	C	C6-N1-C2	-6.45	117.72	120.30
1	A	1010	G	C8-N9-C4	-6.45	103.82	106.40
1	A	1028	C	C6-N1-C2	-6.45	117.72	120.30
1	A	458	C	C6-N1-C2	-6.44	117.72	120.30
1	A	1323	G	N1-C6-O6	6.43	123.76	119.90
1	A	357	G	C5-C6-N1	-6.43	108.29	111.50
1	A	1363	C	C6-N1-C1'	6.41	128.50	120.80
1	A	1007	C	C2-N3-C4	6.41	123.10	119.90
1	A	749	C	C6-N1-C2	-6.41	117.74	120.30
1	A	974	A	N7-C8-N9	6.41	117.00	113.80
1	A	1299	A	C8-N9-C4	-6.41	103.24	105.80
1	A	1224	G	N3-C4-C5	-6.38	125.41	128.60
1	A	496	A	C8-N9-C4	-6.36	103.26	105.80
1	A	911	U	N3-C4-O4	-6.35	114.95	119.40
1	A	44	G	N1-C2-N2	-6.35	110.49	116.20
1	A	357	G	N3-C4-N9	-6.34	122.19	126.00
20	T	10	LEU	N-CA-C	6.34	128.13	111.00
1	A	1502	A	C4-C5-N7	6.34	113.87	110.70
1	A	836	G	C5-C6-O6	-6.34	124.80	128.60
1	A	1334	G	N9-C4-C5	6.33	107.93	105.40
1	A	1029	C	C5-C4-N4	6.33	124.63	120.20
1	A	795	C	N3-C4-C5	-6.33	119.37	121.90
1	A	801	U	C2-N3-C4	-6.33	123.20	127.00
1	A	805	C	C5-C6-N1	6.32	124.16	121.00
1	A	259	G	C5-C6-O6	-6.31	124.81	128.60
1	A	1003	G	C5-C6-O6	6.30	132.38	128.60
1	A	1107	C	C6-N1-C2	-6.30	117.78	120.30
1	A	1269	A	N1-C6-N6	-6.30	114.82	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1417	G	C8-N9-C4	6.30	108.92	106.40
1	A	1199	U	C5-C4-O4	6.29	129.68	125.90
1	A	190	U	C5-C6-N1	6.28	125.84	122.70
1	A	1058	G	C4-C5-N7	6.28	113.31	110.80
1	A	1518	A	N1-C2-N3	6.27	132.43	129.30
1	A	1224	G	C2-N3-C4	6.26	115.03	111.90
1	A	1325	C	C6-N1-C2	6.26	122.80	120.30
1	A	1123	A	N3-C4-C5	6.24	131.17	126.80
1	A	402	G	N3-C2-N2	-6.23	115.54	119.90
1	A	1341	U	C2-N3-C4	-6.23	123.26	127.00
1	A	523	A	C8-N9-C4	-6.22	103.31	105.80
1	A	429	U	C5-C6-N1	-6.22	119.59	122.70
1	A	1160	G	N3-C4-N9	6.22	129.73	126.00
1	A	365	U	N1-C2-N3	6.21	118.63	114.90
1	A	1053	G	C8-N9-C4	6.21	108.89	106.40
1	A	1088	G	N1-C6-O6	6.21	123.62	119.90
1	A	823	G	C8-N9-C4	6.19	108.88	106.40
1	A	1030	C	C5-C6-N1	6.17	124.09	121.00
1	A	47	C	C2-N3-C4	-6.16	116.82	119.90
1	A	992	U	C2-N1-C1'	6.16	125.10	117.70
1	A	92	C	C5-C4-N4	-6.16	115.89	120.20
1	A	358	U	N1-C2-N3	-6.16	111.20	114.90
15	O	17	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	1029	C	N1-C2-O2	6.16	122.59	118.90
1	A	1123	A	N1-C2-N3	-6.16	126.22	129.30
1	A	912	C	C2-N1-C1'	-6.15	112.04	118.80
1	A	1281	U	C6-N1-C2	-6.14	117.31	121.00
1	A	738	C	C6-N1-C2	-6.12	117.85	120.30
1	A	1054	C	N3-C2-O2	-6.12	117.62	121.90
1	A	442	C	C6-N1-C2	-6.11	117.86	120.30
1	A	507	C	C6-N1-C2	-6.11	117.86	120.30
1	A	1504	G	N3-C4-C5	6.10	131.65	128.60
1	A	1442	G	C4-C5-N7	-6.08	108.37	110.80
1	A	42	G	N1-C6-O6	-6.08	116.25	119.90
1	A	52	G	C6-N1-C2	6.06	128.73	125.10
1	A	1305	G	N3-C4-N9	-6.05	122.37	126.00
1	A	1305	G	N9-C4-C5	6.05	107.82	105.40
1	A	754	C	C2-N1-C1'	6.03	125.44	118.80
1	A	1099	G	C5-C6-O6	6.03	132.22	128.60
1	A	1442	G	N7-C8-N9	-6.02	110.09	113.10
1	A	926	G	N1-C6-O6	6.02	123.51	119.90
1	A	44	G	N9-C4-C5	6.01	107.81	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1006	C	C2-N3-C4	6.01	122.91	119.90
1	A	1279	A	C8-N9-C4	-6.01	103.39	105.80
1	A	1390	U	C5-C6-N1	-6.00	119.70	122.70
1	A	850	U	C5-C4-O4	5.98	129.49	125.90
1	A	104	G	C8-N9-C4	5.98	108.79	106.40
1	A	237	C	C5-C6-N1	-5.96	118.02	121.00
1	A	1334	G	C5-C6-O6	5.95	132.17	128.60
1	A	923	A	C8-N9-C4	-5.95	103.42	105.80
1	A	1352	C	C6-N1-C2	-5.95	117.92	120.30
1	A	1338	G	N1-C6-O6	-5.93	116.34	119.90
1	A	1281	U	C2-N1-C1'	5.93	124.81	117.70
1	A	63	C	N1-C2-O2	5.92	122.45	118.90
1	A	921	U	C5-C6-N1	5.92	125.66	122.70
1	A	286	G	N9-C4-C5	5.92	107.77	105.40
1	A	1002	G	C8-N9-C1'	5.92	134.69	127.00
1	A	530	G	C5-N7-C8	-5.92	101.34	104.30
1	A	1224	G	N9-C4-C5	5.90	107.76	105.40
1	A	1504	G	N7-C8-N9	-5.90	110.15	113.10
1	A	921	U	C6-N1-C2	-5.90	117.46	121.00
1	A	43	C	C2-N3-C4	-5.89	116.95	119.90
1	A	1061	G	N3-C2-N2	-5.89	115.78	119.90
1	A	328	C	C5-C6-N1	-5.88	118.06	121.00
1	A	1123	A	C4-C5-C6	-5.87	114.06	117.00
1	A	1299	A	N7-C8-N9	5.87	116.73	113.80
1	A	1363	C	N1-C2-O2	-5.86	115.39	118.90
1	A	1443	G	N1-C2-N3	-5.85	120.39	123.90
1	A	413	G	N3-C4-N9	-5.85	122.49	126.00
1	A	204	U	C2-N1-C1'	5.85	124.72	117.70
1	A	1052	U	N3-C2-O2	-5.85	118.11	122.20
1	A	1520	G	N9-C4-C5	-5.85	103.06	105.40
1	A	1091	U	N1-C2-O2	5.84	126.89	122.80
1	A	1442	G	C8-N9-C4	5.84	108.74	106.40
1	A	1506	U	N3-C2-O2	5.84	126.29	122.20
1	A	1317	C	N3-C2-O2	-5.83	117.82	121.90
1	A	1506	U	N1-C2-O2	-5.83	118.72	122.80
1	A	768	A	C5-C6-N6	-5.83	119.04	123.70
1	A	442	C	C5-C6-N1	5.82	123.91	121.00
1	A	668	G	N1-C6-O6	-5.82	116.41	119.90
1	A	1310	G	C5-C6-O6	-5.81	125.11	128.60
1	A	1404	C	C5-C4-N4	5.81	124.27	120.20
1	A	286	G	C8-N9-C4	-5.81	104.08	106.40
1	A	636	U	N3-C4-O4	5.80	123.46	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	621	A	N9-C4-C5	5.80	108.12	105.80
1	A	39	G	C6-N1-C2	5.80	128.58	125.10
1	A	403	C	N3-C4-N4	5.80	122.06	118.00
1	A	235	C	N3-C2-O2	5.79	125.96	121.90
1	A	1003	G	C6-C5-N7	5.79	133.88	130.40
1	A	366	C	C5-C6-N1	-5.79	118.10	121.00
15	O	54	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	1151	A	N1-C6-N6	-5.78	115.13	118.60
1	A	604	G	C5-C6-N1	-5.77	108.61	111.50
1	A	77	G	C8-N9-C4	5.77	108.71	106.40
1	A	1181	G	N3-C4-N9	-5.77	122.54	126.00
1	A	801	U	N3-C4-C5	5.77	118.06	114.60
1	A	323	U	C5-C4-O4	-5.76	122.44	125.90
1	A	423	G	C5-C6-O6	-5.76	125.14	128.60
1	A	1260	C	C6-N1-C2	-5.76	118.00	120.30
1	A	73	G	C8-N9-C4	5.76	108.70	106.40
1	A	100	C	C6-N1-C2	-5.76	118.00	120.30
1	A	40	C	C2-N3-C4	5.75	122.78	119.90
1	A	768	A	C5-C6-N1	5.75	120.57	117.70
1	A	1374	A	N1-C6-N6	-5.75	115.15	118.60
1	A	1317	C	C6-N1-C2	-5.75	118.00	120.30
1	A	699	C	C6-N1-C2	-5.74	118.00	120.30
1	A	1150	U	C6-N1-C2	-5.74	117.55	121.00
1	A	1305	G	C6-C5-N7	5.74	133.84	130.40
1	A	700	G	C8-N9-C4	5.74	108.69	106.40
1	A	266	G	N1-C6-O6	5.74	123.34	119.90
1	A	912	C	C6-N1-C2	5.73	122.59	120.30
1	A	1160	G	N3-C4-C5	-5.72	125.74	128.60
1	A	1227	A	C5-N7-C8	-5.71	101.04	103.90
1	A	1091	U	C6-N1-C2	-5.69	117.58	121.00
1	A	611	A	C8-N9-C4	5.69	108.08	105.80
1	A	1126	U	C4-C5-C6	-5.68	116.29	119.70
1	A	189(C)	C	C6-N1-C2	-5.68	118.03	120.30
1	A	266	G	C5-N7-C8	-5.68	101.46	104.30
1	A	1244	C	C6-N1-C2	5.67	122.57	120.30
1	A	1459	C	N3-C4-N4	-5.67	114.03	118.00
1	A	1518	A	C5-C6-N1	-5.67	114.87	117.70
1	A	669	U	N3-C2-O2	-5.67	118.23	122.20
1	A	1207	G	C6-C5-N7	5.67	133.80	130.40
1	A	336	C	C5-C6-N1	5.66	123.83	121.00
1	A	1203	C	N1-C2-O2	-5.66	115.50	118.90
1	A	45	U	N3-C4-C5	5.66	117.99	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	769	G	C8-N9-C4	-5.65	104.14	106.40
1	A	330	C	N1-C2-O2	5.64	122.28	118.90
1	A	1502	A	C5-C6-N1	-5.64	114.88	117.70
1	A	365	U	C6-N1-C1'	5.63	129.09	121.20
1	A	1030(B)	C	C6-N1-C2	-5.63	118.05	120.30
1	A	1486	G	N1-C6-O6	5.63	123.28	119.90
1	A	44	G	C8-N9-C4	-5.63	104.15	106.40
1	A	720	C	N1-C2-O2	5.63	122.28	118.90
1	A	1089	G	C4-N9-C1'	-5.62	119.19	126.50
1	A	354	G	N3-C2-N2	-5.62	115.97	119.90
1	A	805	C	C4-C5-C6	-5.62	114.59	117.40
1	A	435	C	C5-C6-N1	5.61	123.81	121.00
1	A	357	G	N3-C2-N2	-5.61	115.97	119.90
1	A	991	U	C6-N1-C2	-5.61	117.64	121.00
1	A	817	C	N1-C2-O2	-5.60	115.54	118.90
1	A	1521	G	C2-N3-C4	5.60	114.70	111.90
1	A	3	G	C4-N9-C1'	5.60	133.78	126.50
1	A	286	G	C5-C6-O6	5.60	131.96	128.60
1	A	530	G	N7-C8-N9	5.60	115.90	113.10
1	A	1058	G	N1-C6-O6	5.60	123.26	119.90
1	A	810	C	C5-C6-N1	-5.59	118.20	121.00
1	A	1366	C	N3-C4-C5	-5.59	119.67	121.90
1	A	1290	G	C4-N9-C1'	5.57	133.74	126.50
1	A	915	A	C5-N7-C8	5.57	106.69	103.90
1	A	1334	G	C8-N9-C4	-5.57	104.17	106.40
1	A	1004	A	N1-C6-N6	-5.56	115.26	118.60
1	A	52	G	C8-N9-C4	-5.56	104.18	106.40
1	A	99	U	N1-C2-O2	-5.55	118.91	122.80
1	A	1197	G	C8-N9-C1'	-5.55	119.78	127.00
1	A	858	G	N7-C8-N9	5.55	115.88	113.10
1	A	773	G	N1-C6-O6	-5.54	116.57	119.90
1	A	860	A	N7-C8-N9	5.54	116.57	113.80
1	A	1442(A)	G	C4-C5-C6	5.54	122.12	118.80
1	A	353	A	N1-C6-N6	5.54	121.92	118.60
1	A	1404	C	N3-C4-N4	-5.54	114.12	118.00
1	A	77	G	N3-C2-N2	5.53	123.77	119.90
1	A	1341	U	N1-C2-N3	5.53	118.22	114.90
1	A	1065	U	N3-C2-O2	-5.53	118.33	122.20
1	A	1282	C	C2-N1-C1'	5.53	124.88	118.80
1	A	425	G	C8-N9-C4	-5.53	104.19	106.40
1	A	52	G	N7-C8-N9	5.52	115.86	113.10
1	A	1282	C	N1-C2-O2	5.52	122.21	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	G	C8-N9-C4	5.52	108.61	106.40
1	A	45	U	N3-C2-O2	-5.51	118.34	122.20
1	A	769	G	N9-C4-C5	5.51	107.61	105.40
1	A	39	G	C2-N3-C4	5.50	114.65	111.90
1	A	942	G	C5-C6-O6	5.50	131.90	128.60
1	A	1030(B)	C	C5-C6-N1	5.50	123.75	121.00
1	A	824	C	C2-N1-C1'	-5.50	112.75	118.80
1	A	1012	U	N1-C2-N3	5.49	118.20	114.90
1	A	1036	G	N3-C2-N2	-5.49	116.06	119.90
1	A	1237	C	C2-N3-C4	-5.48	117.16	119.90
1	A	369	C	C6-N1-C2	-5.48	118.11	120.30
1	A	1468	A	N1-C6-N6	5.47	121.88	118.60
1	A	949	A	C8-N9-C4	-5.46	103.62	105.80
1	A	1177	G	N1-C6-O6	5.44	123.17	119.90
1	A	1468	A	C5-C6-N1	5.43	120.42	117.70
1	A	54	C	C6-N1-C2	-5.43	118.13	120.30
1	A	1151	A	N9-C4-C5	5.43	107.97	105.80
1	A	1150	U	C5-C6-N1	5.42	125.41	122.70
1	A	146	G	C8-N9-C4	-5.42	104.23	106.40
1	A	668	G	N9-C4-C5	5.42	107.57	105.40
1	A	1443	G	C8-N9-C4	5.40	108.56	106.40
1	A	1123	A	N1-C6-N6	-5.40	115.36	118.60
1	A	1089	G	C6-C5-N7	5.40	133.64	130.40
1	A	357	G	N1-C2-N3	-5.39	120.67	123.90
1	A	1481	U	C5-C4-O4	-5.39	122.67	125.90
1	A	530	G	C4-C5-N7	5.39	112.95	110.80
1	A	1510	U	C6-N1-C2	5.39	124.23	121.00
1	A	932	C	C6-N1-C2	-5.38	118.15	120.30
1	A	857	C	C4-C5-C6	5.37	120.08	117.40
1	A	1338	G	C5-C6-O6	5.37	131.82	128.60
1	A	187	C	C2-N1-C1'	5.37	124.70	118.80
1	A	259	G	N1-C6-O6	5.37	123.12	119.90
1	A	355	C	N1-C2-N3	5.36	122.95	119.20
1	A	860	A	C5-N7-C8	-5.36	101.22	103.90
1	A	1322	C	N3-C4-N4	5.36	121.75	118.00
1	A	1506	U	C5-C4-O4	-5.36	122.69	125.90
1	A	1273	G	N3-C4-N9	5.36	129.21	126.00
1	A	328	C	C6-N1-C2	5.35	122.44	120.30
1	A	1107	C	N3-C4-C5	-5.35	119.76	121.90
1	A	722	A	N1-C6-N6	5.34	121.80	118.60
1	A	798	G	C5-C6-O6	5.34	131.80	128.60
1	A	1123	A	C8-N9-C1'	5.34	137.31	127.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	C	N3-C2-O2	-5.34	118.16	121.90
1	A	1279	A	N7-C8-N9	5.34	116.47	113.80
1	A	243	A	C8-N9-C4	-5.34	103.67	105.80
1	A	906	G	C6-C5-N7	-5.34	127.20	130.40
1	A	894	G	N7-C8-N9	-5.33	110.43	113.10
1	A	542	G	C8-N9-C4	-5.33	104.27	106.40
1	A	1226	C	C6-N1-C1'	5.33	127.20	120.80
1	A	57	G	C6-N1-C2	-5.33	121.90	125.10
1	A	1079	G	C8-N9-C4	-5.33	104.27	106.40
1	A	1067	A	P-O3'-C3'	5.33	126.09	119.70
1	A	1016	A	N1-C6-N6	-5.31	115.41	118.60
1	A	913	A	P-O3'-C3'	5.31	126.08	119.70
1	A	1138	G	N3-C4-N9	5.31	129.19	126.00
1	A	1028	C	C5-C6-N1	5.31	123.65	121.00
1	A	1040	U	C2-N1-C1'	-5.31	111.33	117.70
1	A	1052	U	N1-C2-O2	5.31	126.52	122.80
1	A	1518	A	C8-N9-C4	-5.30	103.68	105.80
1	A	1396	A	C5-C6-N6	5.30	127.94	123.70
1	A	766	A	N1-C6-N6	5.29	121.78	118.60
1	A	481	G	N3-C4-C5	-5.29	125.95	128.60
1	A	705	U	N1-C2-O2	-5.29	119.10	122.80
1	A	957	U	N1-C2-O2	5.28	126.50	122.80
1	A	1416	G	C8-N9-C4	-5.28	104.29	106.40
1	A	1305	G	C4-C5-N7	-5.28	108.69	110.80
1	A	423	G	N3-C4-N9	5.28	129.17	126.00
1	A	1125	U	N3-C2-O2	5.28	125.89	122.20
1	A	904	C	N3-C4-C5	-5.27	119.79	121.90
1	A	885	G	C8-N9-C4	5.27	108.51	106.40
1	A	1370	G	C8-N9-C4	-5.26	104.30	106.40
1	A	579	G	C4-C5-C6	5.26	121.95	118.80
1	A	458	C	N3-C4-C5	-5.25	119.80	121.90
1	A	1032	G	C8-N9-C4	-5.25	104.30	106.40
1	A	268	C	C6-N1-C2	-5.25	118.20	120.30
1	A	1224	G	C8-N9-C4	-5.25	104.30	106.40
1	A	810	C	C4-C5-C6	5.25	120.02	117.40
1	A	1440	C	C5-C6-N1	-5.25	118.38	121.00
1	A	1003	G	C4-C5-N7	-5.25	108.70	110.80
1	A	1379	G	N3-C2-N2	-5.25	116.23	119.90
1	A	171	A	C8-N9-C4	-5.24	103.70	105.80
1	A	447	G	N3-C4-N9	5.24	129.14	126.00
1	A	1290	G	N7-C8-N9	5.24	115.72	113.10
1	A	39	G	C4-C5-N7	5.23	112.89	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	560	U	C3'-C2'-C1'	5.23	105.68	101.50
1	A	1330	U	C6-N1-C2	5.23	124.14	121.00
1	A	358	U	N3-C4-C5	-5.22	111.47	114.60
1	A	1443	G	C4-N9-C1'	-5.22	119.71	126.50
1	A	1345	U	C6-N1-C2	5.22	124.13	121.00
1	A	1366	C	C2-N3-C4	5.21	122.51	119.90
1	A	1195	C	C5-C4-N4	5.21	123.85	120.20
1	A	266	G	C4-C5-N7	5.21	112.89	110.80
1	A	927	G	N3-C4-C5	5.21	131.21	128.60
1	A	1480	G	C2-N3-C4	-5.21	109.30	111.90
1	A	1028	C	N1-C2-O2	5.20	122.02	118.90
1	A	479	C	N3-C4-C5	-5.20	119.82	121.90
1	A	1417	G	C5-C6-N1	5.20	114.10	111.50
1	A	43	C	C5-C6-N1	-5.20	118.40	121.00
1	A	841	U	C5-C6-N1	5.20	125.30	122.70
1	A	918	A	C8-N9-C4	-5.20	103.72	105.80
1	A	1123	A	C4-N9-C1'	-5.20	116.94	126.30
1	A	131	C	N3-C2-O2	-5.20	118.26	121.90
1	A	1145	C	C2-N3-C4	5.20	122.50	119.90
1	A	1442(B)	A	N9-C4-C5	5.20	107.88	105.80
1	A	1460	A	C8-N9-C4	5.20	107.88	105.80
1	A	227	G	N3-C2-N2	5.20	123.54	119.90
1	A	365	U	N1-C2-O2	-5.19	119.16	122.80
1	A	524	G	C8-N9-C4	-5.19	104.33	106.40
1	A	1195	C	N3-C2-O2	-5.19	118.27	121.90
1	A	189(B)	C	C6-N1-C2	-5.18	118.23	120.30
1	A	836	G	C8-N9-C1'	-5.18	120.26	127.00
1	A	1231	G	C5-C6-O6	5.18	131.71	128.60
1	A	1443	G	C6-C5-N7	5.18	133.51	130.40
1	A	402	G	C4-C5-C6	5.18	121.91	118.80
1	A	1318	A	C8-N9-C4	-5.18	103.73	105.80
1	A	1017	G	C5-C6-O6	5.18	131.71	128.60
1	A	43	C	N3-C4-N4	-5.18	114.38	118.00
1	A	646	U	C6-N1-C2	-5.18	117.89	121.00
1	A	1330	U	C5-C6-N1	-5.18	120.11	122.70
1	A	916	G	C8-N9-C4	-5.17	104.33	106.40
1	A	43	C	C6-N1-C2	5.17	122.37	120.30
1	A	806	C	C6-N1-C2	-5.17	118.23	120.30
1	A	1002	G	C4-N9-C1'	-5.17	119.78	126.50
1	A	1195	C	N3-C4-N4	-5.17	114.38	118.00
1	A	217	C	C6-N1-C2	5.16	122.37	120.30
1	A	357	G	N1-C6-O6	5.16	123.00	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1235	U	C5-C4-O4	5.16	129.00	125.90
1	A	1269	A	N7-C8-N9	-5.16	111.22	113.80
1	A	1459	C	C6-N1-C1'	-5.16	114.61	120.80
1	A	824	C	C6-N1-C2	5.16	122.36	120.30
1	A	1294	G	C8-N9-C4	-5.15	104.34	106.40
1	A	687	A	C8-N9-C4	-5.15	103.74	105.80
1	A	1338	G	N3-C4-C5	-5.15	126.03	128.60
1	A	297	G	N9-C4-C5	-5.15	103.34	105.40
1	A	1334	G	N1-C6-O6	-5.15	116.81	119.90
1	A	1218	C	N3-C2-O2	-5.14	118.30	121.90
1	A	1303	C	C6-N1-C2	-5.14	118.24	120.30
1	A	1511	G	N9-C4-C5	-5.14	103.34	105.40
1	A	243	A	P-O3'-C3'	5.14	125.87	119.70
1	A	828	A	C8-N9-C4	5.14	107.86	105.80
1	A	1066	C	N3-C2-O2	-5.14	118.31	121.90
1	A	719	C	C4-C5-C6	5.13	119.97	117.40
1	A	1519	A	N7-C8-N9	5.13	116.36	113.80
1	A	1006	C	C5-C6-N1	5.13	123.56	121.00
1	A	1294	G	N3-C4-N9	-5.13	122.92	126.00
1	A	878	G	C8-N9-C4	5.12	108.45	106.40
1	A	1338	G	C8-N9-C4	-5.12	104.35	106.40
1	A	1510	U	N1-C2-N3	-5.12	111.83	114.90
1	A	1396	A	N1-C6-N6	-5.12	115.53	118.60
1	A	974	A	C5-N7-C8	-5.12	101.34	103.90
1	A	1493	A	N7-C8-N9	5.12	116.36	113.80
1	A	974	A	C5-C6-N6	-5.12	119.61	123.70
18	R	31	LEU	CA-CB-CG	5.11	127.06	115.30
1	A	297	G	N3-C4-C5	5.11	131.16	128.60
1	A	1088	G	N3-C4-C5	5.11	131.16	128.60
1	A	687	A	P-O3'-C3'	5.11	125.83	119.70
1	A	904	C	N3-C2-O2	5.10	125.47	121.90
1	A	305	G	C8-N9-C4	5.10	108.44	106.40
1	A	1002	G	N9-C4-C5	5.09	107.44	105.40
1	A	809	G	C8-N9-C4	5.09	108.44	106.40
1	A	259	G	C4-C5-N7	5.09	112.84	110.80
1	A	1040	U	C6-N1-C1'	5.09	128.32	121.20
1	A	70	G	C5-C6-N1	-5.08	108.96	111.50
1	A	1325	C	C5-C6-N1	-5.08	118.46	121.00
1	A	935	A	N1-C6-N6	-5.08	115.55	118.60
1	A	715	A	C8-N9-C4	5.08	107.83	105.80
1	A	1225	A	C6-N1-C2	5.08	121.65	118.60
1	A	1255	G	C5-C6-O6	-5.08	125.55	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1518	A	C4-C5-C6	5.07	119.54	117.00
1	A	77	G	C4-C5-N7	5.07	112.83	110.80
1	A	32	A	C8-N9-C4	-5.07	103.77	105.80
1	A	760	G	N1-C6-O6	5.07	122.94	119.90
1	A	930	C	C2-N1-C1'	-5.07	113.22	118.80
1	A	1123	A	C6-C5-N7	5.07	135.85	132.30
1	A	359	U	N3-C2-O2	5.06	125.74	122.20
1	A	1099	G	C4-C5-N7	-5.06	108.78	110.80
1	A	919	A	C2-N3-C4	5.06	113.13	110.60
1	A	1216	G	C4-N9-C1'	-5.06	119.92	126.50
1	A	801	U	C5-C6-N1	-5.06	120.17	122.70
1	A	428	G	P-O3'-C3'	5.05	125.77	119.70
1	A	39	G	C4-N9-C1'	-5.05	119.93	126.50
1	A	1036	G	C4-N9-C1'	5.05	133.06	126.50
1	A	769	G	N3-C4-C5	-5.04	126.08	128.60
1	A	555	C	N1-C2-O2	-5.04	115.88	118.90
1	A	70	G	C6-N1-C2	5.04	128.12	125.10
1	A	113	G	N1-C6-O6	-5.04	116.88	119.90
1	A	1043	C	C2-N1-C1'	5.03	124.34	118.80
1	A	1331	G	C8-N9-C4	-5.03	104.39	106.40
1	A	922	G	N7-C8-N9	5.03	115.62	113.10
1	A	1519	A	C4-C5-C6	5.03	119.51	117.00
1	A	49	U	N3-C4-O4	-5.02	115.89	119.40
1	A	811	C	C2-N3-C4	-5.02	117.39	119.90
1	A	1037	C	C4-C5-C6	5.02	119.91	117.40
1	A	915	A	C4-C5-N7	-5.01	108.20	110.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
3	C	180	ALA	Peptide
3	C	50	ALA	Peptide
4	D	29	PRO	Peptide
9	I	39	GLY	Peptide
9	I	44	VAL	Peptide
9	I	45	ALA	Peptide
10	J	79	ARG	Peptide
10	J	86	MET	Peptide
10	J	89	ASP	Peptide
13	M	65	LYS	Peptide

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Mol	Chain	Res	Type	Group
13	M	85	GLY	Peptide
18	R	31	LEU	Peptide

## 5.2 Close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32102	0	16201	698	0
2	B	1777	0	1747	75	0
3	C	1450	0	1314	42	0
4	D	1520	0	1406	44	0
5	E	1105	0	1130	37	0
6	F	781	0	741	17	0
7	G	1167	0	1108	34	0
8	H	1045	0	1033	31	0
9	I	852	0	742	47	0
10	J	659	0	552	40	0
11	K	828	0	822	15	0
12	L	909	0	927	29	0
13	M	801	0	743	42	0
14	N	478	0	496	25	0
15	O	724	0	749	23	0
16	P	651	0	638	34	0
17	Q	823	0	891	29	0
18	R	514	0	530	13	0
19	S	560	0	466	31	0
20	T	699	0	746	24	0
21	U	199	0	208	6	0
22	Y	754	0	776	24	0
23	A	223	0	0	0	0
23	D	2	0	0	0	0
23	E	1	0	0	0	0
23	F	1	0	0	0	0
23	I	1	0	0	0	0
23	L	1	0	0	0	0
23	M	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	O	1	0	0	0	0
23	P	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	460	0	0	25	0
25	D	3	0	0	2	0
25	E	2	0	0	0	0
25	F	2	0	0	0	0
25	G	2	0	0	0	0
25	J	1	0	0	0	0
25	K	1	0	0	0	0
25	L	3	0	0	0	0
25	M	1	0	0	0	0
25	O	4	0	0	0	0
25	Q	3	0	0	0	0
25	Y	1	0	0	0	0
All	All	51116	0	33966	1219	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (1219) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:40:C:N4	1:A:402:G:H1	1.47	1.12
1:A:1003:G:H1	1:A:1037:C:H42	1.00	0.97
1:A:1502:A:H2	1:A:1505:G:H1	1.10	0.93
1:A:1025:U:O2	1:A:1036:G:O6	1.86	0.93
1:A:40:C:N3	1:A:402:G:N2	2.16	0.93
1:A:1286:A:H2'	1:A:1287:A:H4'	1.50	0.92
1:A:1005:A:H1'	1:A:1036:G:H22	1.36	0.91
18:R:32:ARG:HA	18:R:69:THR:HG21	1.54	0.89
1:A:503:C:OP2	12:L:116:SER:HB3	1.72	0.88
1:A:1054:C:N4	22:Y:46:GLN:OE1	2.08	0.87
1:A:1356:G:H2'	1:A:1357:A:C8	2.09	0.86
4:D:106:TYR:HD2	4:D:107:ARG:HG2	1.40	0.85
1:A:1128:C:O2'	1:A:1130:A:N7	2.10	0.85
2:B:87:ARG:HE	2:B:233:SER:HB2	1.40	0.85
1:A:1003:G:H1	1:A:1037:C:N4	1.74	0.84
3:C:155:GLY:HA3	3:C:196:LEU:HD12	1.58	0.84
1:A:1503:A:C8	1:A:1531:A:H8	1.95	0.83
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.61	0.83
1:A:1179:A:H4'	9:I:103:THR:HA	1.58	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1459:C:H41	1:A:1461:G:N2	1.78	0.82
22:Y:13:THR:HG23	22:Y:16:ILE:HG23	1.59	0.82
1:A:1321:C:H3'	1:A:1322:C:H5''	1.62	0.81
1:A:1353:G:OP1	21:U:10:ARG:NH1	2.13	0.81
2:B:185:ILE:HG22	2:B:199:TYR:HB2	1.60	0.81
13:M:65:LYS:HA	13:M:66:LEU:HB2	1.64	0.80
1:A:39:G:O6	1:A:403:C:N3	2.13	0.80
1:A:987:G:H1	1:A:1218:C:H42	1.31	0.79
1:A:1442(A):G:C8	1:A:1442(B):A:C2	2.70	0.79
1:A:1011:G:H1	1:A:1018:C:H42	1.28	0.79
2:B:21:ARG:H	2:B:21:ARG:HD2	1.48	0.78
19:S:36:ARG:NH1	19:S:52:TYR:O	2.16	0.78
3:C:12:LEU:HD11	14:N:51:GLY:HA2	1.65	0.78
2:B:69:LEU:HB3	2:B:162:ILE:HG22	1.65	0.78
1:A:171:A:H2'	1:A:172:A:C8	2.19	0.78
1:A:1221:G:OP1	1:A:1320:C:N4	2.17	0.78
1:A:102:G:O2'	1:A:151:A:N3	2.15	0.78
1:A:1441:G:H21	1:A:1459:C:H6	1.29	0.77
1:A:1442:G:N7	1:A:1442(A):G:C6	2.51	0.77
16:P:28:ARG:HH11	16:P:28:ARG:HG2	1.49	0.77
1:A:49:U:O4	1:A:365:U:H5	1.65	0.77
1:A:991:U:O2'	1:A:992:U:OP2	2.03	0.77
10:J:48:THR:HG1	10:J:62:HIS:HD1	1.27	0.77
1:A:974:A:OP2	14:N:29:ARG:NH2	2.18	0.76
1:A:1442:G:N7	1:A:1442(A):G:C5	2.54	0.76
1:A:1338:G:H2'	1:A:1339:A:C8	2.20	0.76
1:A:1090:U:H2'	1:A:1091:U:H6	1.50	0.76
1:A:642:A:N3	8:H:113:SER:OG	2.19	0.76
1:A:1502:A:H2	1:A:1505:G:N1	1.84	0.76
1:A:509:A:OP2	25:A:2083:HOH:O	2.03	0.76
1:A:1441:G:H4'	1:A:1442:G:N7	2.01	0.75
1:A:353:A:H5'	1:A:353:A:H8	1.51	0.75
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.68	0.75
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.67	0.75
4:D:108:LEU:HB3	4:D:110:PHE:HE1	1.52	0.75
1:A:1459:C:C6	1:A:1460:A:N7	2.55	0.74
5:E:100:VAL:O	5:E:107:ARG:NH2	2.20	0.74
1:A:1442:G:O2'	1:A:1442(A):G:OP1	2.03	0.74
1:A:1007:C:N3	1:A:1022:G:O6	2.19	0.74
1:A:559:A:OP1	5:E:126:ARG:NH2	2.20	0.74
1:A:1298:C:H2'	7:G:114:ARG:HH12	1.53	0.74
1:A:1298:C:OP2	7:G:114:ARG:NH2	2.21	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1459:C:N3	1:A:1460:A:N6	2.36	0.73
3:C:15:THR:HG21	3:C:181:ASN:HA	1.71	0.73
3:C:6:HIS:HD2	3:C:8:ILE:H	1.34	0.73
1:A:975:A:H4'	1:A:976:G:H5''	1.71	0.72
1:A:316:G:OP2	1:A:351:G:O2'	2.06	0.72
11:K:86:GLY:N	11:K:112:THR:OG1	2.20	0.72
1:A:1128:C:H5''	9:I:16:ARG:HH12	1.55	0.72
1:A:289:G:OP2	25:A:2116:HOH:O	2.07	0.72
1:A:1356:G:H2'	1:A:1357:A:H8	1.55	0.72
1:A:1226:C:H2'	13:M:103:THR:HB	1.71	0.72
1:A:1002:G:H2'	1:A:1003:G:O4'	1.90	0.71
1:A:1025:U:C2	1:A:1036:G:O6	2.44	0.71
1:A:222:U:H2'	1:A:223:U:C6	2.25	0.71
20:T:72:LEU:HD11	20:T:80:ARG:HD2	1.71	0.71
1:A:1309:G:OP1	13:M:88:ARG:NH1	2.23	0.71
10:J:39:PRO:HA	10:J:70:ARG:HD3	1.70	0.71
1:A:1086:U:H3	1:A:1099:G:H22	1.38	0.71
1:A:1305:G:N1	1:A:1331:G:O2'	2.23	0.71
1:A:1062:U:H2'	1:A:1063:C:C6	2.26	0.71
1:A:1435:G:H2'	1:A:1436:U:C6	2.26	0.71
1:A:67:C:H2'	1:A:68:G:C8	2.26	0.71
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.55	0.70
3:C:35:GLU:OE2	3:C:59:ARG:NH2	2.24	0.70
1:A:673:G:H2'	1:A:674:G:C8	2.26	0.70
18:R:53:ARG:HH21	18:R:60:ALA:N	1.89	0.70
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.07	0.70
7:G:69:VAL:HG12	7:G:100:ALA:HA	1.74	0.70
1:A:1145:C:N4	25:A:2296:HOH:O	2.24	0.70
1:A:266:G:H5'	1:A:268:C:H41	1.56	0.70
1:A:664:G:H22	1:A:741:G:H1	1.40	0.70
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.74	0.70
1:A:470:C:OP2	25:A:2200:HOH:O	2.09	0.69
1:A:1016:A:H2'	1:A:1017:G:O4'	1.92	0.69
20:T:73:HIS:HB3	20:T:74:LYS:HG2	1.74	0.69
13:M:15:VAL:HG22	13:M:43:THR:O	1.91	0.69
1:A:1003:G:N2	1:A:1037:C:N3	2.40	0.69
1:A:548:G:OP1	25:A:2165:HOH:O	2.10	0.69
10:J:44:VAL:HG22	10:J:66:ARG:HD3	1.75	0.69
1:A:785:G:N7	25:A:1971:HOH:O	2.25	0.69
1:A:186:C:H2'	1:A:187:C:H6	1.58	0.69
1:A:1348:U:H4'	9:I:120:ARG:HD2	1.75	0.69
2:B:116:GLU:HA	2:B:119:GLU:HB2	1.73	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1412:C:H2'	1:A:1413:A:C8	2.28	0.68
2:B:194:PRO:O	2:B:196:LEU:N	2.26	0.68
14:N:23:ARG:HD2	14:N:28:GLY:O	1.92	0.68
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.58	0.68
1:A:1108:G:O6	25:A:2280:HOH:O	2.05	0.68
1:A:501:C:OP1	12:L:117:ARG:NH2	2.27	0.68
1:A:1505:G:OP1	25:A:2175:HOH:O	2.11	0.67
2:B:163:PHE:CD2	2:B:185:ILE:HG13	2.28	0.67
10:J:16:LEU:HD21	10:J:70:ARG:HG3	1.76	0.67
1:A:1015:A:H2'	1:A:1016:A:C8	2.29	0.67
1:A:922:G:H4'	5:E:20:GLN:HA	1.76	0.67
1:A:750:G:N3	15:O:23:GLY:HA3	2.08	0.67
1:A:40:C:H42	1:A:402:G:H1	0.73	0.67
1:A:26:A:N1	25:A:1993:HOH:O	2.28	0.67
1:A:457:C:H2'	1:A:458:C:H6	1.59	0.67
1:A:934:C:OP1	25:A:1937:HOH:O	2.12	0.67
1:A:165:C:H2'	1:A:166:G:C8	2.28	0.67
1:A:1457:G:OP1	20:T:39:LYS:NZ	2.28	0.67
2:B:201:ILE:HG21	2:B:214:ILE:HG21	1.75	0.67
1:A:100:C:H2'	1:A:101:A:C8	2.30	0.67
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.77	0.67
7:G:146:GLU:O	7:G:149:ARG:N	2.28	0.67
1:A:735:C:H2'	1:A:736:C:H6	1.59	0.67
8:H:73:ASP:OD2	8:H:75:ARG:HD3	1.94	0.67
1:A:1320:C:H6	1:A:1320:C:H5'	1.60	0.66
6:F:11:ASN:HB3	6:F:14:LEU:HG	1.77	0.66
1:A:1503:A:C8	1:A:1531:A:C8	2.82	0.66
14:N:21:TYR:OH	14:N:23:ARG:NH2	2.27	0.66
20:T:43:LEU:O	20:T:47:GLY:N	2.28	0.66
1:A:1168:A:H2'	1:A:1169:A:C8	2.30	0.66
25:A:2240:HOH:O	11:K:26:ASN:HB3	1.96	0.66
6:F:15:ASP:OD2	6:F:17:SER:N	2.23	0.66
4:D:106:TYR:CD2	4:D:107:ARG:HG2	2.29	0.66
1:A:1459:C:H2'	1:A:1460:A:C8	2.30	0.66
13:M:70:LEU:O	13:M:73:GLU:N	2.29	0.66
9:I:66:ARG:HH11	9:I:66:ARG:HB2	1.60	0.66
1:A:1158:C:H5	1:A:1181:G:H1	1.41	0.66
19:S:31:ILE:HG23	19:S:49:ILE:HG23	1.76	0.66
1:A:266:G:O2'	1:A:267:C:OP2	2.10	0.66
13:M:60:VAL:HG13	13:M:64:TRP:HZ3	1.60	0.66
2:B:87:ARG:NE	2:B:233:SER:HB2	2.11	0.66
1:A:625:G:H4'	16:P:16:HIS:CG	2.31	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1493:A:O2'	1:A:1494:G:OP1	2.13	0.66
1:A:73:G:H1	1:A:96:U:H3	1.42	0.66
1:A:1456:G:O2'	20:T:39:LYS:NZ	2.23	0.65
5:E:144:THR:OG1	5:E:147:ASP:OD2	2.11	0.65
1:A:39:G:N1	1:A:403:C:O2	2.18	0.65
1:A:992:U:O2'	1:A:993:G:O4'	2.12	0.65
1:A:1055:A:O2'	3:C:161:GLU:O	2.15	0.65
2:B:19:HIS:ND1	2:B:189:ASP:OD2	2.21	0.65
1:A:171:A:H2'	1:A:172:A:H8	1.60	0.65
1:A:1164:G:H1	1:A:1172:C:H42	1.44	0.65
2:B:15:VAL:HG23	2:B:209:ARG:HG2	1.77	0.65
1:A:509:A:OP2	25:A:2082:HOH:O	2.15	0.65
14:N:37:PHE:CE1	14:N:53:LEU:HD13	2.32	0.65
2:B:91:PRO:HG2	2:B:155:LEU:HD23	1.78	0.65
9:I:3:GLN:OE1	9:I:20:ARG:NH2	2.29	0.65
5:E:102:ALA:O	5:E:107:ARG:NH1	2.29	0.65
11:K:86:GLY:H	11:K:112:THR:HG1	1.44	0.65
1:A:243:A:H4'	1:A:244:U:O5'	1.97	0.65
13:M:70:LEU:O	13:M:74:VAL:N	2.27	0.65
1:A:608:A:OP2	25:A:2179:HOH:O	2.15	0.65
4:D:108:LEU:HB3	4:D:110:PHE:CE1	2.33	0.64
1:A:982:U:H5''	14:N:6:LEU:HD21	1.80	0.64
1:A:814:A:OP2	25:A:2202:HOH:O	2.14	0.64
1:A:1320:C:C4	19:S:36:ARG:HB2	2.31	0.64
2:B:21:ARG:N	2:B:21:ARG:HD2	2.10	0.64
9:I:45:ALA:HB3	9:I:47:LEU:H	1.62	0.64
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.78	0.64
1:A:946:A:H2'	1:A:947:G:C8	2.32	0.64
1:A:1011:G:H1	1:A:1018:C:N4	1.94	0.64
2:B:163:PHE:HA	2:B:185:ILE:HG12	1.79	0.64
10:J:40:LEU:HB2	10:J:69:ASN:HB2	1.79	0.64
16:P:20:VAL:HG21	16:P:32:TYR:CD1	2.33	0.64
16:P:28:ARG:NH1	16:P:29:ASP:OD2	2.30	0.64
1:A:1441:G:H4'	1:A:1442:G:C8	2.33	0.64
1:A:792:A:OP2	25:A:1978:HOH:O	2.15	0.64
1:A:1442:G:O2'	1:A:1442(A):G:H5'	1.98	0.63
14:N:26:ARG:HD3	14:N:43:CYS:HB3	1.80	0.63
1:A:920:U:H2'	1:A:921:U:C6	2.33	0.63
13:M:50:GLU:HA	13:M:53:VAL:HB	1.81	0.63
1:A:1346:A:H2'	7:G:10:ARG:HH22	1.62	0.63
1:A:1108:G:H5'	3:C:176:HIS:CD2	2.33	0.63
16:P:51:VAL:HG12	16:P:53:VAL:H	1.64	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1237:C:O2'	1:A:1300:G:N2	2.24	0.63
1:A:17:U:H2'	1:A:18:C:C6	2.33	0.63
1:A:1129:C:N4	1:A:1134:G:N7	2.47	0.63
4:D:65:ARG:HG2	4:D:75:PHE:CD1	2.34	0.63
1:A:1030(D):A:H2'	1:A:1031:G:O4'	1.99	0.62
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.14	0.62
1:A:446:G:O6	25:A:2251:HOH:O	2.13	0.62
1:A:1118:C:H1'	1:A:1179:A:C4	2.34	0.62
1:A:1492:A:H5'	1:A:1493:A:C8	2.34	0.62
1:A:186:C:H2'	1:A:187:C:C6	2.35	0.62
1:A:473:G:H2'	1:A:474:G:H8	1.63	0.62
2:B:134:GLU:HA	2:B:137:ARG:HE	1.65	0.62
1:A:1318:A:H1'	19:S:37:ARG:HH21	1.65	0.62
5:E:80:ILE:HD12	5:E:138:ALA:HB1	1.81	0.62
1:A:1010:G:N2	1:A:1020:U:H1'	2.15	0.62
10:J:37:PRO:HA	10:J:72:VAL:HG12	1.82	0.62
2:B:87:ARG:HE	2:B:233:SER:CB	2.13	0.61
1:A:1010:G:H2'	1:A:1011:G:C8	2.34	0.61
1:A:1009:G:H2'	1:A:1010:G:O4'	2.00	0.61
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.33	0.61
4:D:188:LEU:HD23	4:D:188:LEU:H	1.65	0.61
9:I:46:ALA:O	9:I:49:PRO:HD2	2.01	0.61
9:I:21:PRO:HA	9:I:59:PHE:HA	1.83	0.61
19:S:36:ARG:NH2	19:S:75:ALA:O	2.32	0.61
5:E:143:ARG:NH1	8:H:77:GLU:OE1	2.34	0.61
8:H:120:THR:H	8:H:123:GLU:HB2	1.66	0.61
4:D:31:CYS:HB3	4:D:33:MET:HB2	1.83	0.61
1:A:227:G:O2'	16:P:62:VAL:HG22	2.01	0.61
1:A:1029:C:O2	1:A:1032:G:N1	2.34	0.60
1:A:1259:C:N4	1:A:1260:C:O2	2.34	0.60
1:A:91:C:H2'	1:A:92:C:C6	2.37	0.60
1:A:612:C:O2	1:A:629:G:N2	2.33	0.60
9:I:53:VAL:O	9:I:55:ALA:N	2.33	0.60
9:I:8:GLY:HA3	9:I:76:ALA:O	2.01	0.60
1:A:838:G:H2'	1:A:839:U:H5''	1.84	0.60
2:B:18:GLY:HA3	2:B:41:ILE:HD13	1.81	0.60
6:F:82:ARG:HH11	6:F:82:ARG:HG3	1.66	0.60
1:A:600:C:H2'	1:A:601:C:C6	2.36	0.60
1:A:436:C:O2'	1:A:437:U:OP2	2.18	0.60
1:A:828:A:H2'	1:A:829:G:O4'	2.01	0.60
1:A:1342:C:O2'	9:I:124:GLN:HG2	2.00	0.60
1:A:262:A:H2'	1:A:263:A:C8	2.36	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:C:H4'	1:A:172:A:O4'	2.01	0.60
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.83	0.60
16:P:72:ARG:HH21	16:P:73:LEU:HD21	1.67	0.60
2:B:69:LEU:HD13	2:B:91:PRO:HB2	1.84	0.60
3:C:6:HIS:CD2	3:C:8:ILE:H	2.18	0.60
10:J:38:ILE:HG12	10:J:71:LEU:O	2.02	0.60
20:T:10:LEU:HD23	20:T:12:ALA:H	1.66	0.60
16:P:20:VAL:HG23	16:P:35:LYS:HA	1.83	0.59
22:Y:85:LEU:O	22:Y:89:GLN:HG2	2.02	0.59
7:G:37:ASN:OD1	9:I:40:LEU:HA	2.02	0.59
7:G:90:GLU:CD	7:G:90:GLU:H	2.04	0.59
1:A:57:G:H2'	1:A:58:C:C6	2.37	0.59
2:B:115:LEU:HD13	2:B:145:LEU:HB3	1.85	0.59
9:I:9:ARG:HG2	9:I:14:VAL:HG13	1.85	0.59
1:A:869:G:N7	25:A:2204:HOH:O	2.32	0.59
1:A:131:C:H2'	1:A:132:C:H6	1.67	0.59
8:H:87:SER:HA	8:H:93:VAL:HG23	1.84	0.59
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.84	0.59
1:A:987:G:H1	1:A:1218:C:N4	2.01	0.59
1:A:625:G:H4'	16:P:16:HIS:CD2	2.38	0.59
1:A:1117:G:H4'	9:I:104:ARG:NH1	2.16	0.59
10:J:9:ARG:HB2	10:J:95:GLU:HB3	1.85	0.59
1:A:78:G:H1	1:A:91:C:N4	2.01	0.59
1:A:143:A:H2	1:A:220:G:H1	1.51	0.59
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.83	0.59
1:A:1300:G:O2'	1:A:1301:U:O5'	2.21	0.58
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.37	0.58
4:D:158:ILE:O	4:D:162:LEU:N	2.36	0.58
4:D:13:ARG:NH1	4:D:38:TYR:O	2.35	0.58
1:A:1047:G:H5''	14:N:4:LYS:HD3	1.85	0.58
10:J:48:THR:HG1	10:J:62:HIS:CE1	2.21	0.58
1:A:141:A:H1'	1:A:182:U:O2	2.03	0.58
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.86	0.58
1:A:1126:U:OP2	1:A:1281:U:H1'	2.03	0.58
1:A:1070:U:H2'	1:A:1071:C:H6	1.67	0.58
1:A:664:G:P	18:R:64:ARG:HH21	2.27	0.58
3:C:51:GLY:HA3	3:C:71:ALA:HB3	1.86	0.58
1:A:1110:A:OP2	25:A:2210:HOH:O	2.17	0.58
2:B:87:ARG:HH21	2:B:233:SER:HB2	1.66	0.58
5:E:50:GLU:HB2	5:E:53:LEU:HD13	1.84	0.58
1:A:1292:U:O2'	1:A:1293:G:H5'	2.04	0.58
1:A:91:C:O2'	1:A:92:C:H5'	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:228:A:H4'	16:P:62:VAL:HG13	1.84	0.57
1:A:434:U:H2'	1:A:435:C:C6	2.39	0.57
1:A:1203:C:H2'	1:A:1204:A:O4'	2.04	0.57
1:A:974:A:H8	1:A:974:A:OP1	1.87	0.57
3:C:58:GLU:HB2	3:C:65:ALA:HB3	1.85	0.57
1:A:748:C:H4'	1:A:749:C:O5'	2.03	0.57
7:G:38:LEU:O	7:G:42:ILE:HG13	2.03	0.57
1:A:353:A:H5'	1:A:353:A:C8	2.36	0.57
1:A:1400:C:N3	22:Y:63:ALA:HA	2.18	0.57
11:K:79:SER:HA	11:K:104:GLN:HB2	1.87	0.57
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.68	0.57
9:I:89:ASN:O	9:I:91:ASP:N	2.38	0.57
18:R:47:THR:HG23	18:R:49:LYS:HG3	1.86	0.57
1:A:1065:U:H1'	1:A:1066:C:OP2	2.05	0.57
9:I:110:GLU:OE2	9:I:113:LYS:NZ	2.38	0.57
12:L:49:ASN:ND2	12:L:92:ASP:OD2	2.37	0.57
1:A:1005:A:H1'	1:A:1036:G:N2	2.16	0.57
13:M:65:LYS:HA	13:M:66:LEU:CB	2.35	0.57
15:O:5:LYS:O	15:O:9:GLN:HG2	2.04	0.57
9:I:27:THR:HG23	9:I:31:GLN:H	1.69	0.56
1:A:93:G:HO2'	1:A:96:U:H6	1.54	0.56
1:A:933:G:OP2	7:G:3:ARG:HB2	2.04	0.56
10:J:48:THR:OG1	10:J:62:HIS:ND1	2.24	0.56
1:A:1189:C:P	10:J:51:ARG:HH22	2.28	0.56
1:A:1269:A:H2	1:A:1312:G:N3	2.02	0.56
6:F:69:GLU:O	6:F:72:VAL:HG13	2.05	0.56
1:A:228:A:H4'	16:P:62:VAL:CG1	2.36	0.56
1:A:1329:A:P	13:M:28:ALA:HB3	2.45	0.56
1:A:1315:U:H2'	1:A:1316:G:O4'	2.05	0.56
1:A:1009:G:O6	1:A:1020:U:O2	2.24	0.56
13:M:56:LEU:O	13:M:60:VAL:HG23	2.05	0.56
1:A:976:G:H5'	1:A:1358:U:O2'	2.06	0.56
1:A:826:C:H2'	1:A:827:U:C6	2.41	0.56
17:Q:53:LEU:HD23	17:Q:82:MET:HE1	1.87	0.56
1:A:584:G:H5'	17:Q:91:ARG:HH22	1.70	0.56
4:D:173:TRP:CD1	4:D:174:LEU:HG	2.40	0.55
9:I:112:LYS:HE2	9:I:117:HIS:O	2.06	0.55
1:A:1070:U:H2'	1:A:1071:C:C6	2.41	0.55
1:A:1412:C:H2'	1:A:1413:A:H8	1.71	0.55
1:A:620:C:O4'	4:D:135:LEU:HD23	2.07	0.55
18:R:58:LEU:HD12	18:R:62:GLU:OE1	2.06	0.55
1:A:833:U:H2'	1:A:834:C:H6	1.69	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:663:A:O3'	18:R:64:ARG:NH2	2.39	0.55
1:A:1068:G:H8	1:A:1068:G:OP2	1.89	0.55
1:A:1136:U:H5''	1:A:1137:C:C4	2.41	0.55
1:A:131:C:H2'	1:A:132:C:C6	2.41	0.55
2:B:12:GLU:O	2:B:16:HIS:ND1	2.37	0.55
1:A:769:G:H4'	1:A:1513:A:H4'	1.88	0.55
9:I:9:ARG:O	9:I:104:ARG:HG3	2.07	0.55
2:B:87:ARG:HD2	2:B:219:VAL:HG11	1.89	0.55
16:P:28:ARG:HH11	16:P:28:ARG:CG	2.17	0.55
1:A:1181:G:H2'	1:A:1182:G:C5	2.42	0.55
1:A:1207:G:H2'	1:A:1208:C:C6	2.42	0.55
4:D:126:ILE:HG22	4:D:127:THR:H	1.72	0.55
11:K:19:ALA:HB3	11:K:82:VAL:HG22	1.87	0.55
19:S:34:TRP:H	19:S:34:TRP:HE3	1.55	0.55
1:A:674:G:H2'	1:A:675:A:C8	2.42	0.55
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.40	0.55
9:I:45:ALA:CB	9:I:47:LEU:H	2.19	0.55
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.89	0.55
1:A:763:G:H2'	1:A:764:C:H6	1.72	0.55
1:A:671:G:H2'	1:A:672:U:H6	1.72	0.55
20:T:73:HIS:HB3	20:T:74:LYS:HE2	1.89	0.54
1:A:1305:G:N2	1:A:1331:G:O2'	2.40	0.54
1:A:78:G:N2	1:A:91:C:N3	2.54	0.54
1:A:176:C:H2'	1:A:177:C:C6	2.42	0.54
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.42	0.54
1:A:1225:A:N3	1:A:1225:A:H2'	2.22	0.54
1:A:222:U:H2'	1:A:223:U:H6	1.67	0.54
1:A:1307:U:OP1	13:M:101:GLN:NE2	2.33	0.54
7:G:15:ASP:HB3	7:G:24:THR:HG23	1.88	0.54
6:F:76:ALA:O	6:F:80:ARG:HG3	2.08	0.54
1:A:1024:G:O5'	1:A:1024:G:H8	1.90	0.54
1:A:1442(A):G:N7	1:A:1442(B):A:C2	2.76	0.54
1:A:674:G:H2'	1:A:675:A:H8	1.71	0.54
2:B:194:PRO:C	2:B:196:LEU:H	2.11	0.54
1:A:1072:G:H2'	1:A:1073:U:C6	2.42	0.54
5:E:51:VAL:O	5:E:55:VAL:HG23	2.06	0.54
1:A:1223:C:OP2	19:S:78:ARG:NH2	2.40	0.54
1:A:601:C:H2'	1:A:602:A:H8	1.71	0.54
2:B:17:PHE:HB3	2:B:44:LEU:HD11	1.89	0.54
1:A:662:G:H2'	1:A:663:A:C8	2.42	0.54
9:I:43:ALA:O	9:I:45:ALA:HB2	2.07	0.54
1:A:980:C:OP1	25:A:2071:HOH:O	2.18	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:17:THR:HG22	8:H:63:LEU:HG	1.90	0.54
4:D:155:LEU:HD23	4:D:156:GLU:N	2.23	0.54
1:A:373:A:H2'	1:A:374:A:H8	1.73	0.54
16:P:3:LYS:O	16:P:21:VAL:HA	2.08	0.54
1:A:1178:G:N2	1:A:1181:G:OP2	2.40	0.54
10:J:45:ARG:HG2	10:J:47:PHE:CZ	2.41	0.54
1:A:826:C:H2'	1:A:827:U:H6	1.73	0.54
1:A:57:G:H2'	1:A:58:C:H6	1.73	0.54
1:A:57:G:N2	1:A:388:G:C6	2.76	0.54
15:O:8:LYS:HG2	15:O:12:ILE:HD11	1.89	0.54
1:A:228:A:O2'	16:P:2:VAL:HG11	2.07	0.54
1:A:1032:G:H2'	1:A:1033:G:C8	2.43	0.54
19:S:34:TRP:CE3	19:S:34:TRP:N	2.76	0.54
1:A:1202:G:H2'	1:A:1203:C:H5'	1.89	0.54
13:M:15:VAL:O	13:M:19:LEU:HD22	2.07	0.54
1:A:1303:C:H2'	1:A:1304:G:H5'	1.90	0.54
5:E:36:ASP:OD2	5:E:38:GLN:N	2.38	0.54
1:A:975:A:N6	1:A:1367:C:O4'	2.41	0.54
1:A:827:U:H5''	1:A:828:A:OP2	2.07	0.54
3:C:23:TYR:CD1	10:J:10:GLY:HA2	2.43	0.54
19:S:49:ILE:HG13	19:S:62:ILE:HD11	1.89	0.53
1:A:1293:G:HO2'	1:A:1294:G:H8	1.55	0.53
1:A:991:U:H6	1:A:991:U:O5'	1.91	0.53
1:A:56:U:H2'	1:A:57:G:C8	2.44	0.53
3:C:51:GLY:O	3:C:52:LEU:HD22	2.08	0.53
1:A:833:U:H2'	1:A:834:C:C6	2.43	0.53
1:A:859:A:H2'	1:A:860:A:O4'	2.08	0.53
3:C:3:ASN:N	3:C:3:ASN:OD1	2.41	0.53
1:A:601:C:H2'	1:A:602:A:C8	2.43	0.53
1:A:983:A:H2	1:A:984:C:C6	2.26	0.53
1:A:49:U:O4	1:A:365:U:C5	2.54	0.53
3:C:32:LEU:HD13	3:C:59:ARG:HH11	1.72	0.53
1:A:1264:C:H2'	1:A:1265:G:C8	2.44	0.53
2:B:187:LEU:HA	2:B:201:ILE:HB	1.91	0.53
1:A:1166:G:N2	1:A:1169:A:H3'	2.24	0.53
1:A:1319:A:O2'	1:A:1323:G:N7	2.32	0.53
1:A:67:C:H2'	1:A:68:G:H8	1.73	0.53
3:C:6:HIS:HD2	3:C:8:ILE:N	2.04	0.53
1:A:1452:C:O2'	1:A:1456:G:OP2	2.27	0.53
1:A:1457:G:H2'	1:A:1458:G:C8	2.44	0.53
1:A:1258:G:H2'	1:A:1259:C:H6	1.74	0.53
1:A:127:G:HO2'	17:Q:2:PRO:N	2.07	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:24:GLY:HA2	9:I:59:PHE:O	2.09	0.53
22:Y:23:ARG:NH1	22:Y:26:LYS:HD2	2.23	0.53
1:A:270:A:H2'	1:A:271:C:C6	2.43	0.53
1:A:1145:C:H4'	1:A:1146:A:H5'	1.90	0.53
1:A:1149:C:H2'	1:A:1150:U:C6	2.43	0.53
1:A:1223:C:P	19:S:78:ARG:HH21	2.32	0.53
22:Y:23:ARG:HH12	22:Y:26:LYS:HD2	1.73	0.53
8:H:121:ASP:OD1	8:H:121:ASP:N	2.39	0.53
1:A:1126:U:H6	1:A:1280:A:N7	2.05	0.53
1:A:518:C:O2'	1:A:530:G:N2	2.42	0.53
4:D:129:ASN:HD21	4:D:144:ASP:HA	1.74	0.53
1:A:66:G:O4'	1:A:173:U:C4	2.62	0.53
1:A:539:A:H2'	1:A:540:G:C8	2.44	0.52
22:Y:12:ILE:HG21	22:Y:17:ARG:HH21	1.74	0.52
1:A:986:A:H1'	19:S:54:GLY:O	2.09	0.52
1:A:814:A:H2'	1:A:816:A:H5''	1.91	0.52
1:A:1110:A:H8	1:A:1110:A:O5'	1.92	0.52
13:M:87:TYR:O	13:M:90:LEU:N	2.43	0.52
1:A:68:G:O4'	1:A:171:A:H1'	2.10	0.52
5:E:147:ASP:OD2	5:E:147:ASP:N	2.41	0.52
1:A:1414:U:H3	1:A:1486:G:H1	1.55	0.52
1:A:501:C:H2'	1:A:502:G:C8	2.44	0.52
1:A:436:C:O2'	1:A:437:U:P	2.68	0.52
1:A:618:C:N3	1:A:622:A:N6	2.57	0.52
5:E:91:LEU:HD12	5:E:120:THR:HG22	1.90	0.52
4:D:108:LEU:CD1	4:D:174:LEU:HD13	2.39	0.52
1:A:664:G:N2	1:A:741:G:H1	2.07	0.52
1:A:1391:U:H2'	1:A:1392:G:C8	2.44	0.52
1:A:62:U:HO2'	1:A:379:C:C2'	2.19	0.52
1:A:78:G:N1	1:A:91:C:N4	2.58	0.52
1:A:509:A:H3'	1:A:509:A:C8	2.45	0.52
1:A:254:G:OP1	17:Q:67:LYS:O	2.27	0.52
16:P:72:ARG:HE	16:P:73:LEU:HD23	1.74	0.52
15:O:24:SER:OG	15:O:24:SER:O	2.20	0.52
1:A:1125:U:H6	1:A:1125:U:O5'	1.93	0.52
1:A:1459:C:C5	1:A:1460:A:N7	2.77	0.52
9:I:18:PHE:HD1	9:I:62:TYR:HD2	1.58	0.52
1:A:1123:A:O2'	10:J:38:ILE:HG22	2.10	0.51
8:H:13:ILE:O	8:H:17:THR:HG23	2.09	0.51
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.26	0.51
2:B:114:ARG:HD3	2:B:118:LEU:HG	1.92	0.51
1:A:1443:G:O6	1:A:1459:C:O2	2.29	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:67:ALA:HA	20:T:72:LEU:O	2.10	0.51
12:L:7:ILE:O	12:L:11:VAL:HG23	2.10	0.51
17:Q:18:THR:OG1	17:Q:69:LYS:NZ	2.30	0.51
20:T:30:LYS:HA	20:T:33:ILE:HD12	1.91	0.51
1:A:688:G:H2'	1:A:689:C:H6	1.76	0.51
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.92	0.51
1:A:1441:G:N3	1:A:1459:C:C5	2.78	0.51
3:C:11:ARG:HD3	3:C:15:THR:HB	1.92	0.51
1:A:1149:C:H2'	1:A:1150:U:O4'	2.09	0.51
17:Q:22:LEU:HD13	17:Q:41:LYS:HG2	1.92	0.51
1:A:1305:G:N2	1:A:1331:G:H1'	2.26	0.51
1:A:1400:C:C2	22:Y:63:ALA:HA	2.46	0.51
5:E:32:VAL:HB	5:E:58:ALA:HB1	1.92	0.51
2:B:77:ALA:HB1	2:B:165:VAL:HG11	1.91	0.51
1:A:1410:G:H2'	1:A:1411:C:C6	2.44	0.51
1:A:1277:C:HO2'	1:A:1279:A:H8	1.56	0.51
1:A:731:G:H5'	1:A:766:A:H4'	1.93	0.51
1:A:1003:G:C2	1:A:1004:A:H1'	2.46	0.51
18:R:31:LEU:O	18:R:32:ARG:HB2	2.11	0.51
1:A:36:C:O2'	1:A:501:C:OP1	2.29	0.51
4:D:106:TYR:HA	4:D:111:ALA:HB3	1.92	0.51
1:A:1443:G:O6	1:A:1459:C:C2	2.63	0.51
1:A:1207:G:H2'	1:A:1208:C:H6	1.74	0.51
1:A:1164:G:H1	1:A:1172:C:N4	2.08	0.51
21:U:3:LYS:HD3	21:U:14:TRP:HD1	1.75	0.51
1:A:877:C:H5''	8:H:88:LYS:HD3	1.93	0.51
3:C:32:LEU:HD22	3:C:59:ARG:HH12	1.75	0.51
4:D:31:CYS:C	4:D:33:MET:H	2.14	0.51
1:A:1240:U:OP2	7:G:116:ALA:N	2.32	0.51
18:R:70:ILE:O	18:R:74:ARG:HG3	2.11	0.51
1:A:757:U:H2'	1:A:758:G:O4'	2.11	0.51
18:R:53:ARG:HH21	18:R:60:ALA:H	1.57	0.51
1:A:166:G:H2'	1:A:167:G:H8	1.76	0.51
1:A:1292:U:H2'	1:A:1293:G:H8	1.75	0.51
1:A:1486:G:H2'	1:A:1487:G:O4'	2.11	0.51
1:A:260:G:H2'	1:A:261:U:C6	2.46	0.51
1:A:104:G:H4'	1:A:174:C:O4'	2.10	0.51
17:Q:86:GLU:O	17:Q:90:ILE:HG12	2.11	0.51
17:Q:95:TYR:O	17:Q:98:LEU:HB2	2.11	0.51
5:E:145:LYS:O	5:E:149:GLU:HG2	2.11	0.51
1:A:1165:C:H2'	1:A:1166:G:O4'	2.11	0.51
9:I:4:TYR:HB2	9:I:19:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1005:A:C1'	1:A:1036:G:H22	2.18	0.50
1:A:1202:G:C2'	1:A:1203:C:H5'	2.41	0.50
1:A:39:G:C6	1:A:403:C:N3	2.78	0.50
1:A:976:G:C8	1:A:1362:C:N4	2.80	0.50
1:A:658:G:O4'	15:O:22:THR:HB	2.11	0.50
7:G:108:ALA:O	7:G:119:ARG:HD2	2.10	0.50
2:B:55:PHE:O	2:B:59:GLU:N	2.38	0.50
1:A:974:A:OP2	14:N:41:ARG:NH1	2.45	0.50
1:A:1202:G:O4'	14:N:29:ARG:NH1	2.44	0.50
5:E:53:LEU:H	5:E:53:LEU:HD12	1.76	0.50
10:J:7:LYS:H	10:J:97:GLU:HB3	1.76	0.50
10:J:61:GLU:OE1	14:N:58:LYS:NZ	2.33	0.50
13:M:49:THR:O	13:M:52:GLU:N	2.44	0.50
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.46	0.50
19:S:47:HIS:HB2	19:S:62:ILE:HD13	1.92	0.50
2:B:47:THR:O	2:B:51:LEU:N	2.34	0.50
16:P:52:ASP:HB3	16:P:55:ARG:HB2	1.93	0.50
1:A:1343:G:H2'	1:A:1344:C:C6	2.47	0.50
1:A:875:C:O2'	8:H:14:ARG:NH1	2.44	0.50
1:A:116:A:C8	1:A:116:A:OP2	2.65	0.50
1:A:1399:C:C2	1:A:1502:A:N6	2.80	0.50
1:A:1321:C:C3'	1:A:1322:C:H5''	2.38	0.50
1:A:1508:G:H2'	1:A:1509:C:O4'	2.12	0.50
7:G:69:VAL:O	7:G:138:LYS:HG3	2.11	0.50
1:A:624:C:H2'	1:A:625:G:H8	1.77	0.50
16:P:51:VAL:HG12	16:P:53:VAL:N	2.27	0.50
1:A:969:A:OP1	10:J:55:LYS:NZ	2.44	0.50
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.93	0.50
17:Q:76:LEU:HD11	17:Q:78:GLU:O	2.12	0.50
13:M:6:GLY:HA3	13:M:67:GLU:HB2	1.92	0.50
13:M:69:GLU:O	13:M:71:ARG:N	2.44	0.50
1:A:1202:G:C1'	14:N:29:ARG:HH11	2.24	0.50
1:A:1441:G:O2'	1:A:1459:C:N3	2.32	0.50
22:Y:16:ILE:O	22:Y:20:VAL:HG12	2.12	0.50
1:A:1292:U:H2'	1:A:1293:G:C8	2.46	0.50
18:R:45:SER:OG	18:R:47:THR:HG22	2.11	0.50
1:A:1023:G:H3'	1:A:1024:G:C8	2.47	0.50
1:A:519:C:OP2	12:L:50:SER:OG	2.21	0.50
1:A:631:G:H2'	1:A:632:A:C8	2.46	0.50
4:D:15:GLU:OE2	4:D:66:ARG:NH1	2.45	0.50
2:B:74:LYS:NZ	2:B:205:ASP:OD2	2.45	0.50
9:I:19:LEU:O	9:I:59:PHE:HB3	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:82:ARG:HG3	2:B:92:TYR:OH	2.12	0.50
14:N:24:CYS:SG	14:N:25:VAL:N	2.85	0.50
1:A:107:G:H2'	1:A:108:G:O4'	2.12	0.50
10:J:43:ARG:O	10:J:67:THR:HG23	2.11	0.50
1:A:1442:G:C8	1:A:1442(A):G:C5	3.00	0.50
11:K:85:ARG:HE	11:K:111:ASP:HB3	1.77	0.50
1:A:530:G:H3'	1:A:531:U:C5'	2.42	0.50
13:M:5:ALA:C	13:M:7:VAL:H	2.15	0.50
1:A:134:A:H61	16:P:25:ARG:NH1	2.10	0.50
1:A:474:G:H2'	1:A:475:G:H8	1.77	0.50
1:A:441:A:H3'	1:A:442:C:C6	2.46	0.50
16:P:6:LEU:HB3	16:P:17:TYR:CD2	2.47	0.50
1:A:309:G:O2'	1:A:607:A:N1	2.43	0.50
1:A:1074:G:O2'	1:A:1101:A:N1	2.30	0.50
3:C:182:ILE:HA	3:C:202:ILE:O	2.12	0.50
1:A:1003:G:H5''	1:A:1004:A:OP2	2.11	0.49
2:B:162:ILE:HD11	2:B:184:VAL:HG22	1.92	0.49
1:A:1027:C:H2'	1:A:1028:C:C5	2.47	0.49
8:H:83:ILE:HB	8:H:137:VAL:HG13	1.93	0.49
7:G:116:ALA:O	7:G:120:ILE:HG12	2.12	0.49
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.94	0.49
1:A:955:U:O2'	19:S:83:HIS:HD2	1.95	0.49
1:A:1288:A:N1	1:A:1371:G:H1'	2.27	0.49
1:A:1064:G:H4'	1:A:1065:U:OP1	2.10	0.49
1:A:800:G:O6	25:A:2019:HOH:O	2.20	0.49
22:Y:12:ILE:HD11	22:Y:16:ILE:HD11	1.93	0.49
1:A:1320:C:C6	1:A:1320:C:H5'	2.45	0.49
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.94	0.49
1:A:684:A:H2'	1:A:685:G:C8	2.47	0.49
10:J:11:PHE:O	10:J:68:HIS:NE2	2.44	0.49
3:C:6:HIS:CD2	3:C:9:GLY:H	2.30	0.49
2:B:210:SER:O	2:B:214:ILE:HG12	2.12	0.49
1:A:532:A:H2	1:A:1206:G:H21	1.58	0.49
14:N:4:LYS:O	14:N:7:ILE:HG12	2.12	0.49
1:A:1368:G:OP1	25:A:2242:HOH:O	2.19	0.49
9:I:26:VAL:O	9:I:32:ASP:HA	2.13	0.49
1:A:1370:G:C2	1:A:1371:G:C8	3.00	0.49
1:A:1256:A:H5'	1:A:1258:G:C1'	2.42	0.49
6:F:82:ARG:NH1	6:F:82:ARG:HG3	2.26	0.49
1:A:1264:C:H2'	1:A:1265:G:H8	1.78	0.49
2:B:135:GLN:O	2:B:138:LEU:N	2.44	0.49
11:K:44:SER:OG	11:K:47:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1503:A:N7	1:A:1531:A:H8	2.10	0.49
16:P:51:VAL:CG1	16:P:53:VAL:H	2.25	0.49
1:A:1304:G:H1'	1:A:1333:A:H61	1.77	0.49
2:B:87:ARG:NH2	2:B:233:SER:HB2	2.28	0.49
7:G:69:VAL:CG1	7:G:100:ALA:HA	2.42	0.49
1:A:250:A:H4'	1:A:251:G:O5'	2.11	0.49
3:C:154:SER:HB3	3:C:165:THR:HG23	1.94	0.49
7:G:57:GLU:O	7:G:60:LYS:N	2.45	0.49
1:A:939:G:H5''	7:G:102:ARG:NH1	2.28	0.49
1:A:73:G:C6	1:A:97:G:C6	3.00	0.49
8:H:25:ASP:OD2	8:H:60:ARG:HG3	2.13	0.49
1:A:763:G:H2'	1:A:764:C:C6	2.48	0.49
16:P:36:ILE:HD12	16:P:56:ALA:HB2	1.94	0.49
20:T:56:MET:HG3	20:T:57:ARG:N	2.28	0.49
1:A:1003:G:N2	1:A:1038:C:C4	2.80	0.49
1:A:266:G:H5''	1:A:267:C:C5	2.47	0.49
1:A:134:A:N6	16:P:25:ARG:NH1	2.61	0.49
1:A:1079:G:C6	1:A:1080:A:N6	2.80	0.49
1:A:45:U:H2'	1:A:46:G:C8	2.47	0.49
1:A:1210:C:H2'	1:A:1211:U:H5''	1.93	0.49
4:D:94:LEU:HA	4:D:97:LEU:HD12	1.95	0.49
1:A:1313:U:O4	19:S:4:SER:HA	2.13	0.49
20:T:87:LYS:O	20:T:91:LEU:HG	2.13	0.48
1:A:1457:G:H2'	1:A:1458:G:H8	1.78	0.48
1:A:1513:A:H2'	1:A:1514:C:C6	2.48	0.48
5:E:90:VAL:O	5:E:120:THR:HA	2.14	0.48
2:B:47:THR:HA	2:B:202:PRO:HG2	1.95	0.48
16:P:75:ARG:O	16:P:78:GLY:N	2.34	0.48
1:A:1382:C:H2'	1:A:1383:C:C6	2.48	0.48
4:D:30:LYS:C	4:D:32:ALA:H	2.09	0.48
5:E:89:ILE:HD13	5:E:90:VAL:H	1.78	0.48
11:K:99:GLN:HG2	11:K:105:VAL:HG11	1.96	0.48
1:A:738:C:H2'	1:A:739:C:H6	1.79	0.48
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.95	0.48
1:A:1049:U:OP1	14:N:3:ARG:HB3	2.14	0.48
1:A:1346:A:C2'	7:G:10:ARG:HH22	2.27	0.48
1:A:37:U:O2'	1:A:547:A:N1	2.35	0.48
3:C:52:LEU:HA	3:C:70:VAL:HA	1.96	0.48
16:P:68:ASP:O	16:P:71:ARG:HG2	2.13	0.48
2:B:120:ALA:C	2:B:122:PHE:H	2.17	0.48
1:A:973:G:H3'	1:A:974:A:H5''	1.96	0.48
14:N:3:ARG:O	14:N:6:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1157:A:H4'	1:A:1158:C:O5'	2.13	0.48
16:P:21:VAL:O	16:P:33:ILE:HG12	2.13	0.48
1:A:1516:G:H2'	1:A:1518:A:OP2	2.13	0.48
17:Q:84:LEU:O	17:Q:87:LYS:HB2	2.14	0.48
3:C:150:LYS:HB2	3:C:173:VAL:HG21	1.95	0.48
1:A:110:C:H2'	1:A:111:G:O4'	2.13	0.48
13:M:66:LEU:H	13:M:70:LEU:HB2	1.78	0.48
1:A:102:G:H2'	1:A:103:C:H6	1.79	0.48
10:J:62:HIS:HB2	14:N:59:ALA:HB3	1.96	0.48
11:K:85:ARG:HG2	11:K:112:THR:HA	1.95	0.48
1:A:1236:A:H4'	1:A:1304:G:H4'	1.96	0.48
1:A:363:A:N7	12:L:30:ALA:HB1	2.29	0.48
8:H:44:PHE:HE2	8:H:109:ILE:HD12	1.78	0.48
1:A:149:A:O2'	1:A:150:C:H6	1.97	0.48
13:M:88:ARG:HG3	13:M:98:VAL:HG13	1.95	0.48
1:A:1158:C:H5	1:A:1181:G:H22	1.60	0.48
1:A:435:C:N4	1:A:436:C:H41	2.11	0.48
1:A:942:G:H21	9:I:124:GLN:NE2	2.11	0.48
1:A:1325:C:O2'	1:A:1326:C:H5'	2.13	0.48
3:C:16:ARG:NH1	3:C:183:ASP:HA	2.29	0.48
1:A:1003:G:N3	1:A:1004:A:H1'	2.28	0.48
16:P:20:VAL:HG21	16:P:32:TYR:CG	2.49	0.48
1:A:263:A:OP2	20:T:79:ARG:NH1	2.47	0.48
1:A:392:G:H2'	1:A:393:A:C8	2.48	0.48
1:A:552:U:H4'	12:L:86:ARG:HG2	1.96	0.48
1:A:1288:A:O3'	21:U:10:ARG:NH2	2.47	0.48
4:D:65:ARG:HG2	4:D:75:PHE:CE1	2.49	0.48
3:C:51:GLY:HA3	3:C:71:ALA:CB	2.44	0.48
1:A:1092:A:N3	1:A:1183:A:N6	2.61	0.48
1:A:659:U:H2'	1:A:660:G:O4'	2.14	0.48
1:A:1132:C:H2'	1:A:1133:G:C8	2.49	0.48
9:I:99:LEU:HB3	9:I:101:PHE:HD1	1.79	0.48
1:A:1144:G:N2	1:A:1146:A:H62	2.12	0.47
10:J:16:LEU:HD23	10:J:17:ASP:N	2.28	0.47
10:J:68:HIS:CD2	10:J:68:HIS:H	2.32	0.47
1:A:1131:G:H2'	1:A:1132:C:C6	2.49	0.47
20:T:75:ASN:OD1	20:T:75:ASN:N	2.46	0.47
19:S:52:TYR:CE2	19:S:54:GLY:HA2	2.50	0.47
1:A:1158:C:H5	1:A:1181:G:N1	2.09	0.47
3:C:131:ARG:NH1	5:E:50:GLU:HG3	2.29	0.47
1:A:269:C:H2'	1:A:270:A:C8	2.49	0.47
15:O:21:ASP:OD2	15:O:24:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:71:VAL:HG13	2:B:93:VAL:CG2	2.43	0.47
2:B:127:ILE:C	2:B:129:GLU:H	2.18	0.47
1:A:413:G:N2	1:A:428:G:H1'	2.29	0.47
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.49	0.47
21:U:12:LYS:O	21:U:16:GLY:N	2.46	0.47
1:A:1030(A):G:N2	1:A:1032:G:O6	2.47	0.47
1:A:501:C:H1'	1:A:549:C:H1'	1.96	0.47
4:D:110:PHE:H	4:D:110:PHE:HD1	1.60	0.47
1:A:1122:U:C4	1:A:1123:A:N7	2.82	0.47
1:A:687:A:O2'	1:A:688:G:OP2	2.26	0.47
10:J:68:HIS:CD2	10:J:68:HIS:N	2.81	0.47
1:A:527:G:O2'	1:A:535:A:N1	2.35	0.47
2:B:53:ARG:NH2	2:B:198:ASP:O	2.37	0.47
1:A:560:U:H4'	1:A:561:U:O5'	2.15	0.47
1:A:1365:G:C6	1:A:1366:C:C4	3.03	0.47
1:A:77:G:O6	1:A:78:G:C6	2.68	0.47
17:Q:88:TYR:HD2	17:Q:89:LEU:HD23	1.79	0.47
13:M:85:GLY:HA3	19:S:74:PHE:CD1	2.50	0.47
2:B:178:ARG:NH2	8:H:68:ARG:HH22	2.13	0.47
1:A:1298:C:H4'	1:A:1299:A:O4'	2.15	0.47
1:A:765:G:H5''	1:A:766:A:OP1	2.14	0.47
4:D:89:THR:OG1	25:D:403:HOH:O	2.20	0.47
1:A:380:G:N2	1:A:384:G:C5	2.83	0.47
1:A:1442:G:O6	1:A:1442(A):G:O6	2.33	0.47
15:O:17:ARG:HH11	15:O:17:ARG:CG	2.26	0.47
1:A:1456:G:HO2'	20:T:39:LYS:HZ2	1.54	0.47
1:A:1072:G:C5	1:A:1073:U:C4	3.03	0.47
22:Y:23:ARG:HH11	22:Y:23:ARG:HA	1.79	0.47
10:J:6:ILE:HA	10:J:97:GLU:O	2.14	0.47
16:P:52:ASP:OD2	16:P:55:ARG:HG2	2.14	0.47
1:A:939:G:H5''	7:G:102:ARG:CZ	2.44	0.47
1:A:767:A:H2'	1:A:768:A:O4'	2.15	0.47
1:A:1446:U:O2'	1:A:1447:A:H3'	2.15	0.47
19:S:40:ILE:O	19:S:67:VAL:HG13	2.15	0.47
1:A:922:G:C6	1:A:923:A:C6	3.02	0.47
1:A:97:G:O2'	1:A:98:G:H8	1.97	0.47
5:E:144:THR:O	5:E:148:VAL:HG23	2.15	0.47
1:A:1259:C:C4	1:A:1260:C:O2	2.68	0.47
1:A:390:C:H2'	1:A:391:G:C8	2.50	0.47
9:I:18:PHE:CD1	9:I:62:TYR:HD2	2.33	0.47
1:A:1510:U:H2'	1:A:1511:G:C8	2.50	0.47
1:A:1285:A:H4'	1:A:1286:A:O5'	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1021:G:N2	1:A:1022:G:H1'	2.29	0.47
1:A:673:G:N2	1:A:674:G:C2	2.83	0.47
1:A:1300:G:O2'	1:A:1301:U:P	2.73	0.47
16:P:6:LEU:HB3	16:P:17:TYR:HD2	1.79	0.47
11:K:34:ASP:OD2	11:K:37:GLY:N	2.48	0.47
5:E:12:LEU:HB3	5:E:31:LEU:HB2	1.97	0.47
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.50	0.47
1:A:255:G:P	25:A:2243:HOH:O	2.73	0.47
1:A:448:A:P	1:A:485:G:H22	2.37	0.47
2:B:52:GLU:O	2:B:56:ARG:HG2	2.14	0.47
7:G:75:VAL:HA	7:G:87:VAL:O	2.15	0.47
1:A:502:G:OP1	12:L:117:ARG:N	2.48	0.47
1:A:954:G:O6	13:M:104:ARG:NH1	2.48	0.47
1:A:1124:G:O2'	1:A:1126:U:O4	2.30	0.47
1:A:620:C:H2'	1:A:621:A:O4'	2.15	0.47
13:M:4:ILE:HG12	13:M:5:ALA:N	2.30	0.47
1:A:179:A:H2'	1:A:180:U:H6	1.80	0.47
1:A:1057:G:C4	1:A:1204:A:C2	3.04	0.46
1:A:148:G:O2'	1:A:149:A:H5'	2.15	0.46
1:A:149:A:O2'	1:A:150:C:P	2.71	0.46
1:A:68:G:H5'	1:A:171:A:O2'	2.15	0.46
1:A:1206:G:C6	1:A:1207:G:C5	3.03	0.46
1:A:1300:G:HO2'	1:A:1301:U:P	2.37	0.46
1:A:228:A:H5'	16:P:62:VAL:CG2	2.44	0.46
1:A:1446:U:H4'	1:A:1447:A:C5	2.49	0.46
1:A:1232:U:C4	1:A:1233:G:N7	2.83	0.46
1:A:1251:A:H2'	1:A:1252:A:C8	2.50	0.46
13:M:81:LEU:O	13:M:86:CYS:HB3	2.15	0.46
1:A:690:G:C6	1:A:691:G:C6	3.03	0.46
20:T:47:GLY:HA2	20:T:48:LYS:CB	2.45	0.46
1:A:685:G:O2'	1:A:686:U:H5'	2.15	0.46
1:A:1009:G:O2'	1:A:1010:G:H5'	2.15	0.46
1:A:1366:C:H2'	1:A:1367:C:C6	2.49	0.46
7:G:146:GLU:O	7:G:148:ASN:N	2.48	0.46
1:A:1148:U:H2'	1:A:1149:C:O4'	2.15	0.46
1:A:688:G:H2'	1:A:689:C:C6	2.50	0.46
2:B:42:ILE:HG21	2:B:202:PRO:O	2.15	0.46
8:H:11:THR:HG23	8:H:14:ARG:HH12	1.79	0.46
2:B:178:ARG:HH21	8:H:74:PRO:HG3	1.80	0.46
1:A:128:G:O2'	17:Q:3:LYS:HE2	2.16	0.46
1:A:1296:C:H4'	1:A:1302:U:C5	2.50	0.46
2:B:184:VAL:HG12	2:B:197:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:117:G:OP2	25:A:2116:HOH:O	2.21	0.46
9:I:118:LYS:O	9:I:119:ALA:HB3	2.16	0.46
1:A:947:G:O3'	13:M:109:THR:OG1	2.32	0.46
1:A:1333:A:H2'	1:A:1334:G:O4'	2.15	0.46
1:A:1256:A:H5''	1:A:1257:U:OP1	2.16	0.46
1:A:433:C:O2'	1:A:434:U:H5'	2.15	0.46
1:A:392:G:H2'	1:A:393:A:H8	1.80	0.46
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.98	0.46
3:C:19:GLU:O	3:C:40:ARG:NH2	2.48	0.46
2:B:53:ARG:HH12	2:B:199:TYR:HA	1.80	0.46
1:A:149:A:O2'	1:A:150:C:C6	2.68	0.46
1:A:130:A:O2'	1:A:131:C:O5'	2.30	0.46
10:J:61:GLU:OE2	14:N:45:ARG:NE	2.44	0.46
1:A:414:A:H2'	1:A:415:A:H8	1.79	0.46
1:A:1262:C:H2'	1:A:1263:C:C6	2.49	0.46
1:A:194:C:O3'	20:T:68:LYS:HD2	2.16	0.46
4:D:176:LEU:HD12	4:D:177:ASP:H	1.79	0.46
2:B:54:THR:O	2:B:58:ILE:HG13	2.14	0.46
3:C:15:THR:CG2	3:C:181:ASN:HA	2.43	0.46
10:J:35:SER:N	10:J:73:ASP:O	2.48	0.46
1:A:1293:G:O2'	1:A:1294:G:H8	1.99	0.46
1:A:428:G:HO2'	1:A:429:U:P	2.39	0.46
2:B:87:ARG:NH1	2:B:220:ASP:OD1	2.24	0.46
13:M:66:LEU:O	13:M:70:LEU:HB2	2.16	0.46
1:A:254:G:OP1	17:Q:66:SER:OG	2.33	0.46
1:A:868:C:H2'	1:A:869:G:O4'	2.16	0.46
1:A:1277:C:O2'	1:A:1279:A:H1'	2.16	0.46
1:A:542:G:H2'	1:A:543:C:H6	1.80	0.46
4:D:88:VAL:O	4:D:92:VAL:HG23	2.16	0.46
2:B:98:LEU:HA	2:B:98:LEU:HD23	1.80	0.46
1:A:1053:G:C3'	1:A:1054:C:H5'	2.46	0.46
1:A:1200:C:O5'	1:A:1201:A:H3'	2.16	0.46
1:A:1149:C:P	9:I:9:ARG:HH21	2.39	0.46
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.98	0.46
1:A:1096:C:HO2'	1:A:1170:A:HO2'	1.64	0.46
1:A:114:U:H2'	1:A:115:G:C8	2.50	0.46
9:I:119:ALA:O	9:I:120:ARG:HG3	2.15	0.46
1:A:174:C:H2'	1:A:175:C:H6	1.79	0.46
2:B:51:LEU:O	2:B:55:PHE:HD2	1.99	0.46
1:A:191:G:C6	1:A:192:U:N3	2.84	0.46
1:A:413:G:H22	1:A:428:G:H1'	1.80	0.46
1:A:1120:G:H1	1:A:1153:C:H42	1.64	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:Y:87:LYS:O	22:Y:91:LYS:HB2	2.14	0.46
1:A:90:U:H2'	1:A:91:C:C6	2.51	0.46
1:A:942:G:C2	1:A:1342:C:C2	3.04	0.46
1:A:1323:G:H2'	1:A:1324:A:C8	2.50	0.46
1:A:1277:C:HO2'	1:A:1279:A:H1'	1.81	0.46
4:D:100:ARG:HH12	4:D:137:SER:HB3	1.81	0.46
1:A:616:G:C2	1:A:617:G:C8	3.03	0.46
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.16	0.46
6:F:61:LEU:HB3	6:F:63:TYR:HE2	1.80	0.46
1:A:1130:A:C4	1:A:1146:A:C2	3.04	0.45
1:A:1305:G:C2	1:A:1331:G:O2'	2.69	0.45
1:A:434:U:H2'	1:A:435:C:H6	1.81	0.45
2:B:82:ARG:HG3	2:B:92:TYR:CZ	2.51	0.45
1:A:1152:A:H5'	10:J:13:HIS:CG	2.52	0.45
15:O:18:PHE:HB2	15:O:19:PRO:HD2	1.98	0.45
1:A:1442(A):G:N7	1:A:1442(B):A:N1	2.63	0.45
1:A:473:G:H2'	1:A:474:G:C8	2.48	0.45
19:S:37:ARG:HG3	19:S:37:ARG:H	1.41	0.45
8:H:19:VAL:HG23	8:H:21:LYS:HD3	1.97	0.45
10:J:54:PHE:C	10:J:55:LYS:O	2.54	0.45
1:A:1431:C:H2'	1:A:1432:G:O4'	2.16	0.45
2:B:68:ILE:HG12	2:B:161:ALA:HB3	1.97	0.45
10:J:96:ILE:H	10:J:96:ILE:HD12	1.81	0.45
1:A:1227:A:H3'	1:A:1227:A:C8	2.52	0.45
15:O:56:LEU:O	15:O:60:VAL:HG23	2.16	0.45
1:A:1292:U:C2	1:A:1293:G:N7	2.85	0.45
1:A:841:U:C5	1:A:848:C:H1'	2.52	0.45
12:L:54:LYS:HD2	12:L:54:LYS:N	2.31	0.45
3:C:178:LEU:HD13	3:C:178:LEU:HA	1.63	0.45
1:A:1402:C:H2'	1:A:1403:C:O4'	2.16	0.45
1:A:540:G:H2'	1:A:541:G:O4'	2.16	0.45
9:I:99:LEU:HB3	9:I:101:PHE:CD1	2.51	0.45
3:C:19:GLU:HG3	3:C:40:ARG:NH2	2.32	0.45
17:Q:60:ILE:HG12	17:Q:61:GLU:N	2.30	0.45
15:O:26:GLU:HG2	15:O:26:GLU:H	1.31	0.45
19:S:36:ARG:NH2	19:S:72:GLY:O	2.50	0.45
1:A:1086:U:H2'	1:A:1087:G:H8	1.81	0.45
1:A:474:G:H2'	1:A:475:G:C8	2.52	0.45
1:A:622:A:C8	1:A:623:C:C6	3.05	0.45
1:A:1240:U:P	7:G:116:ALA:HB2	2.56	0.45
5:E:31:LEU:HD23	5:E:45:PHE:HB2	1.97	0.45
1:A:1296:C:H4'	1:A:1302:U:C4	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:101:MET:C	2:B:102:LEU:HD12	2.37	0.45
5:E:8:GLU:HA	5:E:33:VAL:O	2.16	0.45
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.51	0.45
13:M:96:LEU:HD13	13:M:97:PRO:HD2	1.97	0.45
1:A:1216:G:OP1	14:N:2:ALA:HA	2.16	0.45
1:A:1305:G:O2'	1:A:1331:G:N2	2.50	0.45
7:G:26:PHE:O	7:G:30:ILE:HG13	2.17	0.45
1:A:952:U:H4'	1:A:964:A:N1	2.32	0.45
19:S:36:ARG:HB3	19:S:72:GLY:HA3	1.99	0.45
13:M:15:VAL:HG23	13:M:41:PRO:HA	1.98	0.45
1:A:1318:A:H4'	19:S:10:PHE:CZ	2.52	0.45
1:A:671:G:H2'	1:A:672:U:C6	2.50	0.45
10:J:55:LYS:O	10:J:56:HIS:CB	2.65	0.45
1:A:35:G:O2'	12:L:118:SER:O	2.23	0.45
13:M:108:ARG:HD3	13:M:108:ARG:HA	1.76	0.45
22:Y:84:GLN:O	22:Y:88:LEU:HG	2.17	0.45
1:A:142:G:H2'	1:A:143:A:H8	1.82	0.45
4:D:162:LEU:HD23	4:D:162:LEU:HA	1.83	0.45
13:M:86:CYS:SG	13:M:86:CYS:O	2.74	0.45
19:S:20:LEU:HD21	19:S:43:GLU:HG2	1.99	0.45
5:E:139:LEU:HD23	5:E:142:LEU:HD11	1.98	0.45
1:A:559:A:H4'	1:A:560:U:H3'	1.99	0.45
20:T:33:ILE:O	20:T:37:SER:OG	2.30	0.45
17:Q:13:ASP:OD1	17:Q:13:ASP:N	2.50	0.45
1:A:21:G:H2'	1:A:22:G:C8	2.52	0.45
1:A:967:C:O5'	1:A:967:C:H6	1.99	0.45
1:A:165:C:H2'	1:A:166:G:H8	1.77	0.45
8:H:11:THR:HG23	8:H:14:ARG:NH1	2.32	0.45
1:A:44:G:H2'	1:A:45:U:O4'	2.16	0.45
1:A:790:A:C2	22:Y:29:LYS:HD3	2.52	0.45
1:A:721:G:H4'	1:A:722:A:O4'	2.16	0.45
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.72	0.45
1:A:1002:G:C2	1:A:1003:G:H1'	2.52	0.44
1:A:373:A:C2	1:A:374:A:C8	3.05	0.44
17:Q:57:VAL:HG12	17:Q:76:LEU:HD12	1.98	0.44
16:P:71:ARG:O	16:P:75:ARG:N	2.44	0.44
1:A:195:A:C6	1:A:196:A:N1	2.85	0.44
1:A:1441:G:N2	1:A:1459:C:C6	2.81	0.44
1:A:1226:C:OP1	13:M:91:ARG:NH1	2.50	0.44
1:A:1300:G:O2'	1:A:1301:U:H6	1.99	0.44
1:A:397:A:N3	1:A:397:A:H3'	2.32	0.44
4:D:120:LEU:HB3	4:D:126:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:939:G:H2'	1:A:940:C:C6	2.52	0.44
11:K:99:GLN:HG2	11:K:105:VAL:HG21	1.99	0.44
17:Q:24:GLU:OE2	17:Q:37:LYS:HD3	2.16	0.44
4:D:10:ARG:HG3	4:D:11:LEU:HD12	1.98	0.44
1:A:77:G:O6	1:A:78:G:N1	2.50	0.44
1:A:814:A:N7	1:A:816:A:C4	2.85	0.44
1:A:858:G:O6	1:A:869:G:H3'	2.17	0.44
1:A:965:A:OP2	22:Y:8:LYS:NZ	2.51	0.44
17:Q:88:TYR:CD2	17:Q:89:LEU:HD23	2.53	0.44
1:A:909:A:H2'	1:A:910:C:O4'	2.18	0.44
3:C:12:LEU:HD23	3:C:12:LEU:HA	1.86	0.44
1:A:750:G:C2	15:O:23:GLY:HA3	2.52	0.44
1:A:391:G:C6	1:A:392:G:C5	3.05	0.44
1:A:428:G:O2'	1:A:429:U:OP2	2.30	0.44
1:A:1162:C:H2'	1:A:1163:C:C6	2.52	0.44
16:P:67:THR:H	16:P:70:ALA:HB3	1.82	0.44
1:A:951:G:C6	1:A:1231:G:C6	3.05	0.44
1:A:1366:C:H2'	1:A:1367:C:H6	1.82	0.44
1:A:625:G:H2'	1:A:626:U:H6	1.82	0.44
6:F:75:LEU:O	6:F:79:LEU:HG	2.17	0.44
1:A:455:C:H6	1:A:455:C:O5'	2.00	0.44
1:A:36:C:OP1	12:L:123:LYS:NZ	2.50	0.44
1:A:1442(A):G:C5	1:A:1442(B):A:C6	3.06	0.44
1:A:10:A:OP2	5:E:126:ARG:HD2	2.17	0.44
1:A:76:C:O2'	1:A:77:G:OP1	2.30	0.44
1:A:519:C:H2'	1:A:520:A:C8	2.52	0.44
13:M:4:ILE:HG12	13:M:5:ALA:H	1.81	0.44
4:D:94:LEU:O	4:D:97:LEU:HB2	2.18	0.44
5:E:57:LYS:HB3	5:E:61:TYR:CE2	2.53	0.44
1:A:67:C:H4'	1:A:172:A:C4'	2.48	0.44
1:A:1318:A:H4'	19:S:10:PHE:CE1	2.52	0.44
1:A:832:C:O2'	1:A:833:U:P	2.76	0.44
17:Q:45:HIS:HB2	17:Q:65:ILE:HD13	2.00	0.44
10:J:47:PHE:CZ	14:N:37:PHE:HE2	2.36	0.44
2:B:133:LYS:O	2:B:137:ARG:HG3	2.17	0.44
9:I:49:PRO:O	9:I:52:ALA:HB3	2.17	0.44
10:J:96:ILE:H	10:J:96:ILE:CD1	2.29	0.44
1:A:891:U:OP1	25:A:2090:HOH:O	2.21	0.44
12:L:71:PRO:O	12:L:102:ARG:NH1	2.48	0.44
1:A:64:G:H4'	1:A:65:U:H3'	1.99	0.44
15:O:31:LEU:HD23	15:O:31:LEU:HA	1.58	0.44
1:A:1201:A:H4'	1:A:1202:G:O5'	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1179:A:O3'	9:I:103:THR:OG1	2.23	0.44
1:A:750:G:H21	15:O:23:GLY:HA3	1.83	0.44
4:D:83:SER:HA	25:D:403:HOH:O	2.18	0.44
1:A:63:C:H4'	1:A:380:G:H4'	1.99	0.44
13:M:96:LEU:O	13:M:110:ARG:HD3	2.17	0.44
5:E:81:GLU:HB3	5:E:88:LYS:HE2	2.00	0.44
1:A:624:C:H2'	1:A:625:G:C8	2.53	0.43
1:A:1055:A:N6	1:A:1206:G:C5	2.86	0.43
1:A:1031:G:H2'	1:A:1032:G:O4'	2.18	0.43
22:Y:23:ARG:HH12	22:Y:26:LYS:CD	2.30	0.43
1:A:380:G:C2	1:A:384:G:C6	3.06	0.43
2:B:84:GLU:OE1	2:B:216:SER:HA	2.18	0.43
1:A:51:A:C2	1:A:353:A:N1	2.86	0.43
4:D:173:TRP:CE3	4:D:193:ASP:HB3	2.54	0.43
4:D:188:LEU:CD2	4:D:188:LEU:H	2.27	0.43
1:A:262:A:C6	1:A:263:A:C6	3.05	0.43
1:A:1244:C:C2	1:A:1294:G:N2	2.85	0.43
8:H:49:GLU:O	8:H:51:VAL:HG13	2.17	0.43
22:Y:23:ARG:HD2	22:Y:23:ARG:HA	1.81	0.43
1:A:1077:G:N2	1:A:1080:A:OP2	2.50	0.43
1:A:881:G:P	12:L:12:ARG:HH22	2.41	0.43
15:O:15:PHE:CE2	15:O:84:LYS:HD2	2.52	0.43
1:A:1053:G:H3'	1:A:1054:C:H5'	1.99	0.43
1:A:624:C:O3'	16:P:10:GLY:HA2	2.17	0.43
2:B:189:ASP:OD1	2:B:205:ASP:HB3	2.18	0.43
1:A:1281:U:H2'	1:A:1281:U:H6	1.59	0.43
1:A:104:G:H4'	1:A:174:C:C4'	2.49	0.43
1:A:192:U:H4'	20:T:57:ARG:HD2	2.00	0.43
1:A:552:U:H4'	12:L:87:GLY:O	2.17	0.43
1:A:911:U:OP2	12:L:97:ARG:NH1	2.52	0.43
6:F:8:ILE:HD12	6:F:26:ILE:HD13	2.00	0.43
1:A:1004:A:N7	1:A:1036:G:N1	2.67	0.43
1:A:1054:C:H41	22:Y:45:PRO:HB2	1.84	0.43
1:A:78:G:N2	1:A:92:C:N3	2.67	0.43
1:A:1029:C:N3	1:A:1032:G:O6	2.51	0.43
15:O:18:PHE:CD1	15:O:18:PHE:C	2.91	0.43
1:A:841:U:H6	1:A:841:U:OP1	2.01	0.43
4:D:8:VAL:HG22	4:D:21:LEU:CD1	2.48	0.43
1:A:708:C:H2'	1:A:709:G:H8	1.84	0.43
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.99	0.43
1:A:580:U:H2'	1:A:581:G:O4'	2.19	0.43
15:O:3:ILE:HD13	15:O:3:ILE:H	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1530:G:OP1	1:A:1530:G:H4'	2.18	0.43
1:A:962:C:H2'	1:A:963:G:O4'	2.18	0.43
17:Q:22:LEU:HD11	17:Q:39:SER:HB2	1.99	0.43
1:A:174:C:H2'	1:A:175:C:C6	2.53	0.43
1:A:22:G:H4'	1:A:885:G:C8	2.54	0.43
5:E:59:GLY:O	5:E:62:ALA:HB3	2.17	0.43
20:T:18:GLN:O	20:T:22:ARG:HG3	2.18	0.43
1:A:1349:A:C2	1:A:1374:A:C4	3.06	0.43
1:A:199:G:O2'	1:A:200:G:H5'	2.18	0.43
7:G:126:ASP:HB3	7:G:131:LYS:O	2.19	0.43
1:A:958:A:C6	1:A:959:A:C6	3.06	0.43
1:A:7:G:H5'	1:A:298:A:O4'	2.18	0.43
1:A:203:U:OP2	1:A:203:U:H2'	2.19	0.43
1:A:1285:A:H8	1:A:1285:A:O5'	2.02	0.43
1:A:101:A:O2'	1:A:102:G:H5'	2.19	0.43
1:A:1158:C:C4	1:A:1160:G:C5	3.06	0.43
4:D:126:ILE:HG22	4:D:127:THR:N	2.34	0.43
13:M:3:ARG:HG3	13:M:4:ILE:HB	2.00	0.43
1:A:659:U:C2'	1:A:660:G:H5'	2.48	0.43
1:A:926:G:C6	22:Y:87:LYS:HG3	2.54	0.43
1:A:1041:A:H2'	1:A:1042:G:O4'	2.19	0.43
1:A:696:A:H1'	1:A:786:G:O2'	2.19	0.43
1:A:1029:C:O2	1:A:1033:G:C6	2.72	0.43
1:A:1126:U:O2	1:A:1127:G:C5	2.72	0.43
1:A:984:C:H2'	1:A:985:C:H6	1.83	0.43
1:A:738:C:H2'	1:A:739:C:C6	2.53	0.43
1:A:516:U:C4	1:A:517:G:C6	3.06	0.43
4:D:149:ALA:O	4:D:152:SER:OG	2.19	0.43
1:A:1442(A):G:O2'	1:A:1442(B):A:H2'	2.18	0.43
1:A:1353:G:C2	1:A:1370:G:C2	3.07	0.43
2:B:36:ARG:O	2:B:39:ILE:N	2.51	0.43
1:A:992:U:O4	1:A:1044:A:N7	2.52	0.43
8:H:119:LEU:HB3	8:H:123:GLU:HB2	2.01	0.43
6:F:36:ARG:HH11	6:F:36:ARG:CB	2.31	0.43
1:A:1001:A:O5'	1:A:1001:A:H8	2.02	0.43
1:A:1285:A:H4'	1:A:1286:A:C5'	2.49	0.43
1:A:955:U:O2'	19:S:83:HIS:CD2	2.72	0.43
1:A:1309:G:OP2	13:M:99:ARG:NH2	2.44	0.43
1:A:923:A:H2'	1:A:924:C:O4'	2.18	0.43
1:A:1316:G:N2	1:A:1318:A:H3'	2.34	0.43
1:A:815:A:N7	1:A:1509:C:O2'	2.30	0.43
1:A:1142:G:H2'	1:A:1143:G:O4'	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:523:A:H61	12:L:53:ARG:NH1	2.17	0.43
20:T:55:ILE:O	20:T:58:LYS:N	2.52	0.43
1:A:224:C:H2'	1:A:225:C:C6	2.53	0.43
1:A:68:G:C4'	1:A:171:A:H1'	2.48	0.42
1:A:1090:U:H2'	1:A:1091:U:C6	2.40	0.42
1:A:857:C:H2'	1:A:858:G:O4'	2.19	0.42
2:B:12:GLU:O	2:B:16:HIS:HB2	2.18	0.42
1:A:1151:A:O2'	1:A:1152:A:H8	2.02	0.42
1:A:438:G:O2'	1:A:494:U:O4	2.29	0.42
2:B:215:LEU:HA	2:B:215:LEU:HD23	1.73	0.42
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.86	0.42
1:A:1063:C:H3'	1:A:1064:G:H2'	2.01	0.42
1:A:1300:G:C6	1:A:1334:G:C5	3.07	0.42
1:A:228:A:H5'	16:P:62:VAL:HG22	2.00	0.42
10:J:8:LEU:HA	10:J:95:GLU:O	2.18	0.42
1:A:1124:G:H5'	10:J:35:SER:OG	2.19	0.42
8:H:21:LYS:O	8:H:63:LEU:HD23	2.19	0.42
1:A:1504:G:OP1	1:A:1507:A:H4'	2.20	0.42
17:Q:57:VAL:HA	17:Q:77:VAL:HG23	2.00	0.42
3:C:16:ARG:HH12	3:C:183:ASP:HA	1.84	0.42
15:O:74:ASP:HA	15:O:75:PRO:HD2	1.84	0.42
1:A:358:U:H2'	1:A:359:U:C6	2.53	0.42
1:A:1375:A:C6	1:A:1376:U:C4	3.07	0.42
2:B:50:GLU:OE1	2:B:200:ILE:HG12	2.19	0.42
1:A:1400:C:O3'	22:Y:80:LYS:HD3	2.19	0.42
1:A:1080:A:H5''	5:E:16:THR:HG21	2.02	0.42
1:A:321:A:C2	1:A:333:G:C2	3.07	0.42
1:A:102:G:H2'	1:A:103:C:C6	2.55	0.42
20:T:72:LEU:HD23	20:T:73:HIS:N	2.34	0.42
1:A:1346:A:C8	1:A:1348:U:C2	3.08	0.42
9:I:27:THR:HG23	9:I:31:GLN:N	2.35	0.42
17:Q:44:ALA:HA	17:Q:71:PHE:O	2.20	0.42
1:A:189(C):C:H2'	1:A:189(D):C:O4'	2.19	0.42
1:A:1007:C:N3	1:A:1022:G:C6	2.86	0.42
1:A:1158:C:C4	1:A:1160:G:C4	3.08	0.42
1:A:1170:A:C8	1:A:1171:G:C8	3.08	0.42
1:A:1394:A:C5	1:A:1501:C:H4'	2.54	0.42
11:K:62:GLN:HG3	11:K:97:ALA:HB2	2.01	0.42
6:F:91:VAL:HG12	6:F:92:LYS:O	2.20	0.42
2:B:54:THR:HG23	2:B:199:TYR:HB3	2.01	0.42
1:A:1492:A:OP1	12:L:47:LYS:HE3	2.19	0.42
19:S:12:ASP:OD1	19:S:37:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:600:C:H2'	1:A:601:C:H6	1.81	0.42
1:A:373:A:N3	1:A:374:A:C8	2.88	0.42
2:B:42:ILE:HD13	2:B:203:GLY:HA2	2.02	0.42
1:A:520:A:N1	1:A:536:C:H1'	2.35	0.42
1:A:1349:A:C2	1:A:1374:A:C5	3.08	0.42
20:T:92:LEU:O	20:T:96:GLY:HA2	2.19	0.42
1:A:1118:C:H1'	1:A:1179:A:C5	2.55	0.42
1:A:945:G:C2	1:A:946:A:C8	3.08	0.42
9:I:40:LEU:H	9:I:40:LEU:HD23	1.84	0.42
1:A:1379:G:C6	1:A:1380:U:C4	3.07	0.42
1:A:1392:G:O5'	1:A:1392:G:H8	2.03	0.42
19:S:20:LEU:HD21	19:S:43:GLU:CG	2.50	0.42
10:J:50:ILE:HA	10:J:60:ARG:HG2	2.02	0.42
12:L:27:LEU:C	12:L:29:GLY:H	2.23	0.42
2:B:9:GLU:O	2:B:11:LEU:N	2.53	0.42
1:A:1465:C:H2'	1:A:1466:C:O4'	2.19	0.42
5:E:95:ALA:HB1	5:E:96:PRO:HD2	2.01	0.42
1:A:1442(A):G:C4	1:A:1442(B):A:C4	3.08	0.42
1:A:1442:G:O2'	1:A:1442(A):G:P	2.77	0.42
1:A:97:G:O2'	1:A:98:G:H5''	2.19	0.42
7:G:111:ARG:HB3	7:G:113:GLU:HG2	2.02	0.42
6:F:22:GLU:OE2	6:F:82:ARG:HG2	2.20	0.42
6:F:61:LEU:HB3	6:F:63:TYR:CE2	2.54	0.42
4:D:22:LYS:HG3	4:D:26:CYS:SG	2.59	0.42
1:A:1388:C:H2'	1:A:1389:C:C6	2.55	0.42
12:L:124:LYS:HA	12:L:125:PRO:HD3	1.92	0.42
3:C:54:ARG:HG2	3:C:55:VAL:N	2.35	0.42
1:A:1366:C:O2'	1:A:1367:C:H5'	2.19	0.42
1:A:663:A:H2'	1:A:664:G:O4'	2.20	0.42
8:H:97:VAL:O	8:H:100:ILE:HG13	2.20	0.42
14:N:44:LEU:O	14:N:44:LEU:HD12	2.19	0.42
11:K:27:ASN:OD1	11:K:28:THR:N	2.47	0.42
1:A:1442(A):G:C5	1:A:1442(B):A:C5	3.08	0.42
1:A:1226:C:H4'	19:S:80:TYR:OH	2.19	0.42
1:A:947:G:N2	1:A:1235:U:O2	2.53	0.42
4:D:189:PRO:CB	4:D:194:LEU:HD11	2.49	0.42
9:I:19:LEU:HD23	9:I:19:LEU:HA	1.68	0.42
1:A:56:U:H2'	1:A:57:G:H8	1.83	0.42
13:M:6:GLY:HA3	13:M:67:GLU:HG3	2.02	0.42
9:I:28:VAL:HA	9:I:63:ILE:O	2.19	0.42
3:C:148:GLY:HA3	3:C:172:ARG:O	2.20	0.42
3:C:22:TRP:CH2	14:N:54:PRO:HG2	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1496:C:H2'	1:A:1497:G:O4'	2.20	0.42
1:A:1005:A:O2'	1:A:1036:G:N2	2.53	0.41
1:A:993:G:H4'	1:A:994:A:OP2	2.19	0.41
2:B:119:GLU:HG2	2:B:153:ARG:HH22	1.85	0.41
4:D:36:ARG:HG2	4:D:38:TYR:CZ	2.54	0.41
5:E:31:LEU:HD22	5:E:43:LEU:HD11	2.01	0.41
17:Q:13:ASP:O	17:Q:15:MET:N	2.53	0.41
1:A:1003:G:C6	1:A:1004:A:C2	3.08	0.41
1:A:1054:C:N4	22:Y:45:PRO:HB2	2.34	0.41
1:A:1052:U:O4	1:A:1200:C:C2	2.73	0.41
4:D:173:TRP:NE1	4:D:174:LEU:HG	2.35	0.41
14:N:6:LEU:HD23	14:N:23:ARG:HH12	1.84	0.41
8:H:51:VAL:HG11	8:H:60:ARG:HH11	1.85	0.41
1:A:1378:C:C5	1:A:1379:G:C8	3.08	0.41
12:L:24:VAL:HG12	12:L:26:ALA:HB2	2.02	0.41
1:A:1426:C:H2'	1:A:1427:U:C6	2.55	0.41
7:G:48:LYS:O	7:G:52:GLU:HG2	2.20	0.41
5:E:127:ASN:HA	5:E:128:PRO:HD3	1.88	0.41
20:T:64:ASP:OD1	20:T:81:LYS:NZ	2.48	0.41
1:A:1490:C:H2'	1:A:1491:G:O4'	2.20	0.41
1:A:1005:A:C6	1:A:1025:U:H1'	2.55	0.41
10:J:45:ARG:HB3	10:J:65:LEU:HB3	2.02	0.41
1:A:1028:C:C2	1:A:1033:G:N2	2.88	0.41
1:A:939:G:H5''	7:G:102:ARG:NH2	2.35	0.41
6:F:61:LEU:HD23	6:F:63:TYR:OH	2.20	0.41
18:R:33:ASP:OD1	18:R:36:ASN:HB2	2.21	0.41
1:A:189(F):U:O2	17:Q:63:ARG:NH2	2.53	0.41
1:A:112:G:H4'	1:A:389:A:H4'	2.02	0.41
1:A:502:G:P	12:L:116:SER:HA	2.60	0.41
1:A:1503:A:C5	1:A:1531:A:H8	2.38	0.41
2:B:92:TYR:HE1	2:B:94:ASN:HB2	1.85	0.41
10:J:46:ARG:NE	10:J:64:GLU:OE1	2.54	0.41
15:O:57:LEU:HD23	15:O:57:LEU:HA	1.84	0.41
1:A:3:G:N3	1:A:3:G:H2'	2.36	0.41
1:A:953:G:C4	1:A:1229:A:C2	3.08	0.41
1:A:1226:C:H4'	1:A:1227:A:OP1	2.21	0.41
4:D:155:LEU:HD23	4:D:156:GLU:H	1.85	0.41
21:U:3:LYS:HD3	21:U:14:TRP:CD1	2.55	0.41
1:A:940:C:OP1	7:G:29:LYS:NZ	2.53	0.41
1:A:706:A:H2'	1:A:707:C:H5'	2.02	0.41
2:B:164:VAL:HB	2:B:186:ALA:HB2	2.02	0.41
1:A:105:G:H2'	1:A:106:C:C6	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:586:C:C2'	1:A:587:G:H5'	2.51	0.41
1:A:954:G:H2'	1:A:955:U:O4'	2.20	0.41
9:I:65:VAL:O	9:I:66:ARG:HG3	2.21	0.41
1:A:73:G:C6	1:A:76:C:C4	3.09	0.41
1:A:532:A:H5'	25:A:2294:HOH:O	2.19	0.41
14:N:40:CYS:SG	14:N:43:CYS:CB	2.99	0.41
1:A:66:G:O4'	1:A:173:U:C5	2.74	0.41
2:B:71:VAL:O	2:B:165:VAL:HG23	2.20	0.41
1:A:429:U:H4'	1:A:430:A:O5'	2.21	0.41
1:A:293:G:C6	1:A:294:U:C4	3.08	0.41
2:B:27:LYS:HD2	2:B:193:ASP:OD1	2.21	0.41
12:L:85:ILE:HD13	12:L:85:ILE:HA	1.70	0.41
1:A:954:G:OP1	22:Y:17:ARG:NH2	2.53	0.41
22:Y:12:ILE:CG2	22:Y:17:ARG:HE	2.33	0.41
1:A:1493:A:C2	1:A:1494:G:C8	3.08	0.41
1:A:433:C:C2'	1:A:434:U:H5'	2.51	0.41
1:A:1292:U:N3	1:A:1293:G:N7	2.69	0.41
1:A:756:C:H2'	1:A:757:U:O4'	2.21	0.41
1:A:691:G:H2'	1:A:692:U:C6	2.55	0.41
6:F:10:LEU:HD21	6:F:61:LEU:HD22	2.03	0.41
1:A:1310:G:H5'	13:M:77:ASN:ND2	2.35	0.41
13:M:65:LYS:O	13:M:70:LEU:HG	2.20	0.41
1:A:741:G:H2'	1:A:742:G:O4'	2.21	0.41
17:Q:67:LYS:O	17:Q:68:ARG:HB3	2.20	0.41
1:A:1256:A:H5'	1:A:1258:G:H1'	2.03	0.41
1:A:270:A:H2'	1:A:271:C:H6	1.86	0.41
1:A:411:A:C6	1:A:429:U:C4	3.09	0.41
2:B:56:ARG:O	2:B:60:ASP:HB2	2.21	0.41
5:E:57:LYS:HB3	5:E:61:TYR:HE2	1.84	0.41
1:A:1250:A:H4'	9:I:68:GLY:N	2.36	0.41
1:A:163:C:H2'	1:A:164:U:O4'	2.20	0.41
1:A:719:C:C2	18:R:50:ILE:HG12	2.56	0.41
1:A:954:G:H21	1:A:1227:A:H62	1.68	0.41
13:M:73:GLU:O	13:M:76:ALA:HB3	2.21	0.41
1:A:1218:C:H2'	1:A:1219:U:C6	2.55	0.41
1:A:994:A:N7	1:A:1216:G:H4'	2.36	0.41
3:C:32:LEU:HD22	3:C:59:ARG:NH1	2.35	0.41
9:I:46:ALA:HB2	9:I:74:ILE:HG22	2.02	0.41
1:A:984:C:H2'	1:A:985:C:C6	2.56	0.41
13:M:87:TYR:C	13:M:89:GLY:N	2.74	0.41
1:A:938:A:N6	1:A:939:G:C6	2.89	0.41
1:A:881:G:OP2	12:L:12:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:27:LEU:CB	12:L:33:ARG:HD3	2.51	0.41
12:L:32:PHE:HB3	12:L:84:LEU:HD11	2.03	0.41
2:B:25:ASN:O	2:B:27:LYS:N	2.53	0.41
22:Y:93:GLU:C	22:Y:95:ARG:H	2.22	0.41
21:U:9:ARG:O	21:U:13:ILE:HG13	2.21	0.41
9:I:16:ARG:HB2	9:I:64:THR:CG2	2.51	0.41
19:S:75:ALA:HA	19:S:76:PRO:HD3	1.90	0.41
1:A:1091:U:C2	1:A:1095:U:N3	2.89	0.41
1:A:561:U:O2'	1:A:562:C:P	2.80	0.41
1:A:561:U:HO2'	1:A:562:C:P	2.43	0.41
1:A:9:G:H5''	5:E:126:ARG:HD3	2.03	0.41
3:C:6:HIS:HA	3:C:7:PRO:HD3	1.64	0.41
1:A:167:G:O2'	1:A:168:G:H5'	2.20	0.41
1:A:475:G:C2'	1:A:476:G:H5'	2.51	0.41
1:A:142:G:H2'	1:A:143:A:C8	2.56	0.41
1:A:834:C:H2'	1:A:835:U:C6	2.56	0.41
1:A:751:U:H4'	15:O:24:SER:HB2	2.03	0.41
1:A:657:G:C2	1:A:658:G:C8	3.08	0.41
1:A:965:A:H5'	1:A:969:A:O4'	2.21	0.41
1:A:611:A:H2	1:A:630:G:H22	1.69	0.41
1:A:53:A:N1	1:A:54:C:C2	2.89	0.41
6:F:86:ARG:O	6:F:87:ARG:HG2	2.20	0.41
1:A:152:A:N6	1:A:170:U:C2	2.89	0.40
1:A:785:G:C2'	1:A:786:G:H5'	2.51	0.40
4:D:188:LEU:HA	4:D:189:PRO:HD3	1.97	0.40
5:E:143:ARG:HD2	5:E:143:ARG:HH11	1.76	0.40
1:A:1024:G:P	1:A:1024:G:H8	2.44	0.40
12:L:7:ILE:HA	12:L:7:ILE:HD13	1.88	0.40
1:A:1030(B):C:H2'	1:A:1030(C):G:H5'	2.03	0.40
1:A:723:U:H2'	1:A:723:U:H6	1.73	0.40
1:A:1503:A:N9	1:A:1531:A:H8	2.19	0.40
1:A:232:G:H1'	1:A:262:A:N1	2.36	0.40
1:A:1410:G:H2'	1:A:1411:C:H6	1.85	0.40
8:H:14:ARG:O	8:H:18:ARG:HD3	2.21	0.40
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.85	0.40
12:L:84:LEU:HD22	12:L:85:ILE:H	1.84	0.40
11:K:48:ILE:HD11	11:K:64:ALA:HA	2.03	0.40
1:A:593:G:C2	1:A:647:C:O2	2.74	0.40
1:A:40:C:C2	1:A:402:G:N2	2.81	0.40
1:A:1492:A:H2'	1:A:1492:A:N3	2.36	0.40
12:L:47:LYS:HA	12:L:48:PRO:HA	1.80	0.40
1:A:1329:A:OP1	13:M:28:ALA:HB3	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:55:LYS:HG2	10:J:56:HIS:N	2.36	0.40
3:C:180:ALA:HB1	3:C:182:ILE:HG13	2.04	0.40
4:D:30:LYS:CB	4:D:35:ARG:HD2	2.51	0.40
3:C:125:GLU:HG2	3:C:189:ALA:HB1	2.04	0.40
7:G:41:ARG:H	7:G:41:ARG:HG3	1.43	0.40
1:A:1004:A:N7	1:A:1036:G:C2	2.90	0.40
2:B:21:ARG:HB3	2:B:39:ILE:HG12	2.02	0.40
1:A:1452:C:HO2'	1:A:1456:G:P	2.42	0.40
20:T:10:LEU:CG	20:T:11:SER:H	2.35	0.40
1:A:1380:U:C2	7:G:3:ARG:NH1	2.90	0.40
1:A:1101:A:H4'	1:A:1102:A:O5'	2.22	0.40
3:C:150:LYS:HB2	3:C:150:LYS:HE3	1.83	0.40
19:S:74:PHE:CD2	19:S:74:PHE:N	2.89	0.40
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.56	0.40
1:A:257:G:H2'	1:A:258:G:O4'	2.21	0.40
1:A:954:G:C6	1:A:955:U:N3	2.90	0.40
1:A:735:C:H2'	1:A:736:C:C6	2.46	0.40
1:A:1291:G:C5	1:A:1292:U:C5	3.09	0.40
15:O:9:GLN:HA	15:O:12:ILE:HD12	2.02	0.40
1:A:1060:C:O2'	10:J:56:HIS:HD2	2.04	0.40
2:B:92:TYR:CE1	2:B:94:ASN:HB2	2.57	0.40
7:G:29:LYS:HD3	7:G:29:LYS:HA	1.96	0.40
8:H:39:LEU:O	8:H:44:PHE:N	2.53	0.40
11:K:84:VAL:HG11	11:K:91:ARG:HD2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	227/256 (89%)	185 (82%)	40 (18%)	2 (1%)	25	55
3	C	204/239 (85%)	176 (86%)	28 (14%)	0	100	100
4	D	206/209 (99%)	186 (90%)	20 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	146/162 (90%)	128 (88%)	17 (12%)	1 (1%)	30	62
6	F	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	G	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	30	62
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	I	123/128 (96%)	108 (88%)	13 (11%)	2 (2%)	14	35
10	J	94/105 (90%)	72 (77%)	15 (16%)	7 (7%)	2	1
11	K	112/129 (87%)	103 (92%)	9 (8%)	0	100	100
12	L	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	27	58
13	M	112/126 (89%)	86 (77%)	22 (20%)	4 (4%)	5	11
14	N	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	14	33
15	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	P	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	18	43
17	Q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	22	51
18	R	66/88 (75%)	55 (83%)	11 (17%)	0	100	100
19	S	79/93 (85%)	67 (85%)	11 (14%)	1 (1%)	18	43
20	T	94/106 (89%)	77 (82%)	17 (18%)	0	100	100
21	U	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
22	Y	93/119 (78%)	85 (91%)	7 (8%)	1 (1%)	21	49
All	All	2405/2657 (90%)	2107 (88%)	275 (11%)	23 (1%)	22	51

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	56	HIS
13	M	84	ILE
7	G	147	ALA
10	J	55	LYS
10	J	57	LYS
13	M	10	PRO
16	P	53	VAL
19	S	47	HIS
9	I	45	ALA
9	I	54	ASP
12	L	26	ALA
22	Y	95	ARG
2	B	10	LEU

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Mol	Chain	Res	Type
10	J	30	SER
10	J	94	VAL
5	E	146	ALA
17	Q	14	LYS
13	M	66	LEU
14	N	59	ALA
10	J	75	ILE
13	M	7	VAL
2	B	194	PRO
10	J	34	VAL

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	177/220 (80%)	148 (84%)	29 (16%)	3	9
3	C	114/188 (61%)	97 (85%)	17 (15%)	4	11
4	D	139/181 (77%)	119 (86%)	20 (14%)	5	12
5	E	108/123 (88%)	95 (88%)	13 (12%)	7	17
6	F	77/90 (86%)	66 (86%)	11 (14%)	5	12
7	G	104/127 (82%)	91 (88%)	13 (12%)	7	16
8	H	103/119 (87%)	87 (84%)	16 (16%)	4	10
9	I	62/99 (63%)	53 (86%)	9 (14%)	5	12
10	J	52/92 (56%)	41 (79%)	11 (21%)	1	4
11	K	81/99 (82%)	73 (90%)	8 (10%)	11	26
12	L	92/109 (84%)	83 (90%)	9 (10%)	12	26
13	M	63/101 (62%)	46 (73%)	17 (27%)	1	2
14	N	46/50 (92%)	38 (83%)	8 (17%)	3	7
15	O	77/80 (96%)	64 (83%)	13 (17%)	3	8
16	P	63/74 (85%)	50 (79%)	13 (21%)	2	5
17	Q	94/97 (97%)	82 (87%)	12 (13%)	6	15
18	R	49/77 (64%)	40 (82%)	9 (18%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	43/80 (54%)	37 (86%)	6 (14%)	5	12
20	T	62/82 (76%)	53 (86%)	9 (14%)	5	12
21	U	18/22 (82%)	15 (83%)	3 (17%)	3	8
22	Y	82/104 (79%)	70 (85%)	12 (15%)	5	11
All	All	1706/2214 (77%)	1448 (85%)	258 (15%)	4	11

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	24	TRP
2	B	67	THR
2	B	74	LYS
2	B	75	LYS
2	B	80	ILE
2	B	87	ARG
2	B	93	VAL
2	B	97	TRP
2	B	111	ARG
2	B	126	GLU
2	B	139	LYS
2	B	150	SER
2	B	158	LEU
2	B	160	ASP
2	B	170	GLU
2	B	175	ARG
2	B	185	ILE
2	B	187	LEU
2	B	198	ASP
2	B	200	ILE
2	B	205	ASP
2	B	221	LEU
2	B	224	GLN
2	B	231	GLU
2	B	233	SER
3	C	3	ASN
3	C	15	THR
3	C	32	LEU

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Mol	Chain	Res	Type
3	C	49	SER
3	C	52	LEU
3	C	59	ARG
3	C	69	HIS
3	C	70	VAL
3	C	102	ASN
3	C	104	GLN
3	C	111	LEU
3	C	131	ARG
3	C	144	SER
3	C	175	LEU
3	C	178	LEU
3	C	184	TYR
3	C	196	LEU
4	D	8	VAL
4	D	15	GLU
4	D	19	LEU
4	D	28	SER
4	D	36	ARG
4	D	53	ASP
4	D	58	LEU
4	D	65	ARG
4	D	83	SER
4	D	106	TYR
4	D	120	LEU
4	D	122	ARG
4	D	127	THR
4	D	135	LEU
4	D	137	SER
4	D	158	ILE
4	D	170	VAL
4	D	188	LEU
4	D	194	LEU
4	D	196	LEU
5	E	12	LEU
5	E	31	LEU
5	E	34	VAL
5	E	41	VAL
5	E	47	LYS
5	E	65	ASN
5	E	76	ILE
5	E	78	HIS

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Mol	Chain	Res	Type
5	E	89	ILE
5	E	91	LEU
5	E	137	GLU
5	E	144	THR
5	E	147	ASP
6	F	15	ASP
6	F	36	ARG
6	F	40	VAL
6	F	55	ASP
6	F	64	GLN
6	F	69	GLU
6	F	70	ASP
6	F	75	LEU
6	F	86	ARG
6	F	89	MET
6	F	98	LEU
7	G	12	LEU
7	G	15	ASP
7	G	32	ARG
7	G	41	ARG
7	G	51	GLN
7	G	75	VAL
7	G	95	ARG
7	G	98	SER
7	G	104	LEU
7	G	113	GLU
7	G	138	LYS
7	G	144	MET
7	G	146	GLU
8	H	21	LYS
8	H	25	ASP
8	H	26	VAL
8	H	29	SER
8	H	52	ASP
8	H	63	LEU
8	H	78	GLN
8	H	83	ILE
8	H	84	ARG
8	H	85	ARG
8	H	109	ILE
8	H	112	LEU
8	H	115	SER

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Mol	Chain	Res	Type
8	H	121	ASP
8	H	127	LEU
8	H	133	LEU
9	I	14	VAL
9	I	31	GLN
9	I	40	LEU
9	I	64	THR
9	I	66	ARG
9	I	88	TYR
9	I	104	ARG
9	I	107	ARG
9	I	108	VAL
10	J	16	LEU
10	J	21	GLN
10	J	35	SER
10	J	54	PHE
10	J	55	LYS
10	J	67	THR
10	J	68	HIS
10	J	94	VAL
10	J	96	ILE
10	J	97	GLU
10	J	100	THR
11	K	16	SER
11	K	31	THR
11	K	48	ILE
11	K	84	VAL
11	K	96	ARG
11	K	104	GLN
11	K	109	VAL
11	K	114	VAL
12	L	33	ARG
12	L	43	VAL
12	L	53	ARG
12	L	60	LEU
12	L	67	THR
12	L	80	HIS
12	L	83	VAL
12	L	84	LEU
12	L	97	ARG
13	M	3	ARG
13	M	4	ILE

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Mol	Chain	Res	Type
13	M	14	ARG
13	M	15	VAL
13	M	19	LEU
13	M	47	ASP
13	M	49	THR
13	M	56	LEU
13	M	64	TRP
13	M	66	LEU
13	M	69	GLU
13	M	70	LEU
13	M	71	ARG
13	M	78	ILE
13	M	86	CYS
13	M	96	LEU
13	M	110	ARG
14	N	8	GLU
14	N	18	VAL
14	N	22	THR
14	N	24	CYS
14	N	25	VAL
14	N	33	VAL
14	N	44	LEU
14	N	50	LYS
15	O	3	ILE
15	O	10	LYS
15	O	17	ARG
15	O	24	SER
15	O	26	GLU
15	O	35	ARG
15	O	39	LEU
15	O	41	GLU
15	O	65	ARG
15	O	66	LEU
15	O	73	GLU
15	O	76	GLU
15	O	83	GLU
16	P	1	MET
16	P	2	VAL
16	P	20	VAL
16	P	28	ARG
16	P	32	TYR
16	P	33	ILE

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Mol	Chain	Res	Type
16	P	38	TYR
16	P	45	THR
16	P	47	ASP
16	P	62	VAL
16	P	67	THR
16	P	69	THR
16	P	76	GLN
17	Q	9	VAL
17	Q	13	ASP
17	Q	49	GLU
17	Q	50	LYS
17	Q	53	LEU
17	Q	60	ILE
17	Q	62	SER
17	Q	68	ARG
17	Q	74	LEU
17	Q	77	VAL
17	Q	82	MET
17	Q	86	GLU
18	R	21	LYS
18	R	29	PHE
18	R	31	LEU
18	R	32	ARG
18	R	58	LEU
18	R	76	LEU
18	R	82	THR
18	R	85	LEU
18	R	86	VAL
19	S	7	LYS
19	S	14	HIS
19	S	31	ILE
19	S	34	TRP
19	S	37	ARG
19	S	66	MET
20	T	10	LEU
20	T	13	LEU
20	T	24	LEU
20	T	37	SER
20	T	39	LYS
20	T	56	MET
20	T	73	HIS
20	T	75	ASN

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Mol	Chain	Res	Type
20	T	84	LEU
21	U	9	ARG
21	U	10	ARG
21	U	15	ARG
22	Y	13	THR
22	Y	16	ILE
22	Y	20	VAL
22	Y	23	ARG
22	Y	24	LEU
22	Y	41	LEU
22	Y	42	SER
22	Y	44	GLU
22	Y	53	THR
22	Y	76	GLU
22	Y	77	LEU
22	Y	95	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	40	HIS
3	C	6	HIS
3	C	176	HIS
4	D	129	ASN
6	F	73	ASN
7	G	28	ASN
9	I	73	GLN
9	I	124	GLN
10	J	56	HIS
11	K	99	GLN
15	O	28	GLN
16	P	14	ASN
16	P	16	HIS
19	S	83	HIS
22	Y	31	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1490/1522 (97%)	306 (20%)	32 (2%)



All (306) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G
1	A	48	C
1	A	50	A
1	A	51	A
1	A	59	A
1	A	61	G
1	A	67	C
1	A	77	G
1	A	78	G
1	A	79	G
1	A	91	C
1	A	92	C
1	A	93	G
1	A	96	U
1	A	97	G
1	A	115	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	131	C
1	A	144	G
1	A	145	G
1	A	146	G
1	A	150	C
1	A	156	G
1	A	163	C
1	A	173	U
1	A	182	U
1	A	189(G)	G
1	A	195	A
1	A	197	A
1	A	203	U
1	A	204	U
1	A	216	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	266	G

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Mol	Chain	Res	Type
1	A	267	C
1	A	289	G
1	A	306	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	388	G
1	A	391	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	437	U
1	A	439	A
1	A	441	A
1	A	442	C
1	A	452	A
1	A	458	C
1	A	461	A
1	A	476	G
1	A	485	G
1	A	495	A
1	A	496	A
1	A	498	U
1	A	505	G

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Mol	Chain	Res	Type
1	A	506	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	536	C
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	588	G
1	A	596	C
1	A	617	G
1	A	623	C
1	A	630	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	666	G
1	A	673	G
1	A	687	A
1	A	688	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	749	C
1	A	755	G
1	A	764	C
1	A	777	A
1	A	793	U
1	A	794	A
1	A	817	C

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Mol	Chain	Res	Type
1	A	821	G
1	A	827	U
1	A	828	A
1	A	829	G
1	A	833	U
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	853	G
1	A	859	A
1	A	860	A
1	A	902	G
1	A	913	A
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	937	A
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	989	C
1	A	992	U
1	A	993	G
1	A	1000	U
1	A	1002	G
1	A	1003	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1007	C
1	A	1009	G

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Mol	Chain	Res	Type
1	A	1010	G
1	A	1011	G
1	A	1022	G
1	A	1023	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1029	C
1	A	1030	C
1	A	1030(A)	G
1	A	1030(B)	C
1	A	1030(C)	G
1	A	1032	G
1	A	1033	G
1	A	1034	G
1	A	1036	G
1	A	1037	C
1	A	1044	A
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1081	G
1	A	1082	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1133	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G

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Mol	Chain	Res	Type
1	A	1140	C
1	A	1146	A
1	A	1147	C
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1161	C
1	A	1166	G
1	A	1168	A
1	A	1180	A
1	A	1181	G
1	A	1182	G
1	A	1189	C
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1203	C
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1225	A
1	A	1227	A
1	A	1230	C
1	A	1236	A
1	A	1238	A
1	A	1240	U
1	A	1249	C
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1273	G
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1290	G

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Mol	Chain	Res	Type
1	A	1294	G
1	A	1297	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1320	C
1	A	1321	C
1	A	1322	C
1	A	1323	G
1	A	1331	G
1	A	1346	A
1	A	1347	G
1	A	1353	G
1	A	1359	C
1	A	1360	A
1	A	1363	C
1	A	1364	U
1	A	1370	G
1	A	1381	U
1	A	1397	C
1	A	1398	A
1	A	1406	U
1	A	1416	G
1	A	1419	G
1	A	1442	G
1	A	1442(A)	G
1	A	1442(B)	A
1	A	1443	G
1	A	1447	A
1	A	1452	C
1	A	1456	G
1	A	1457	G
1	A	1459	C
1	A	1460	A
1	A	1461	G
1	A	1487	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1502	A

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Mol	Chain	Res	Type
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1508	G
1	A	1517	G
1	A	1519	A
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	60	A
1	A	76	C
1	A	115	G
1	A	119	A
1	A	189(E)	U
1	A	243	A
1	A	266	G
1	A	428	G
1	A	429	U
1	A	495	A
1	A	509	A
1	A	560	U
1	A	561	U
1	A	687	A
1	A	748	C
1	A	913	A
1	A	991	U
1	A	1064	G
1	A	1065	U
1	A	1067	A
1	A	1126	U
1	A	1129	C
1	A	1136	U
1	A	1165	C
1	A	1201	A

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Mol	Chain	Res	Type
1	A	1285	A
1	A	1300	G
1	A	1442	G
1	A	1456	G
1	A	1493	A
1	A	1530	G

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 235 ligands modelled in this entry, 235 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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