



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:00 PM GMT

PDB ID : 3V24  
Title : Crystal structure of RMF bound to the 70S ribosome. This PDB entry contains coordinates for the 30S subunit with bound RMF of the 2nd ribosome in the ASU  
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.  
Deposited on : 2011-12-11  
Resolution : 3.00 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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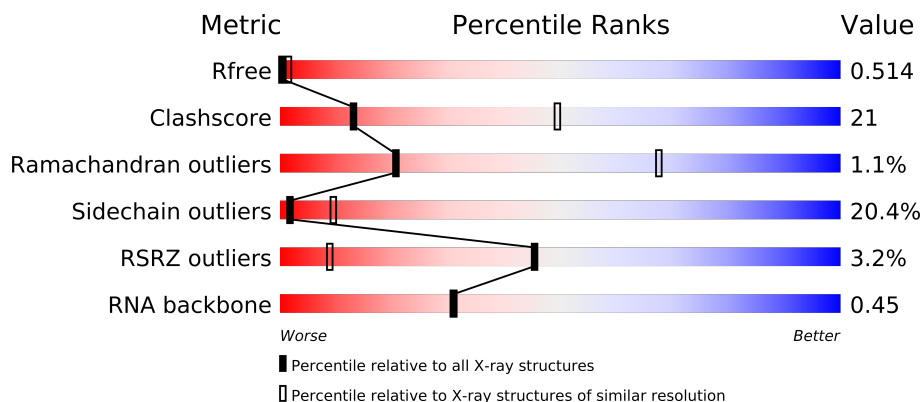
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 Å.

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



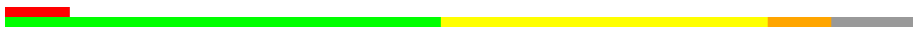
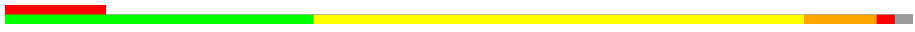



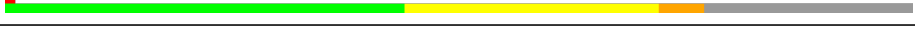




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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.

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	

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Mol	Chain	Length	Quality of chain
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	61	

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 50378 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	1501	Total	C	N	O	P	0	0	0
			32270	14362	5983	10424	1501			

- 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
			1775	1132	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
			1526	963	283	274	6			

- 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
			777	493	137	144	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
			1164	726	224	208	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
			663	410	132	121			

- 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
			905	567	178	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
			804	497	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	97	Total	C	N	O	S	0	0	0
			713	438	152	121	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 modulation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	53	Total	C	N	O	S	0	0	0
			353	218	67	66	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	56	HIS	-	EXPRESSION TAG	UNP P0AFW2
V	57	HIS	-	EXPRESSION TAG	UNP P0AFW2
V	58	HIS	-	EXPRESSION TAG	UNP P0AFW2
V	59	HIS	-	EXPRESSION TAG	UNP P0AFW2
V	60	HIS	-	EXPRESSION TAG	UNP P0AFW2
V	61	HIS	-	EXPRESSION TAG	UNP P0AFW2

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	71	Total	Mg	0	0
			71	71		

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

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	120	Total	O	0	0
			120	120		
25	D	1	Total	O	0	0
			1	1		
25	K	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	P	1	Total	O	0	0
			1	1		
25	T	2	Total	O	0	0
			2	2		

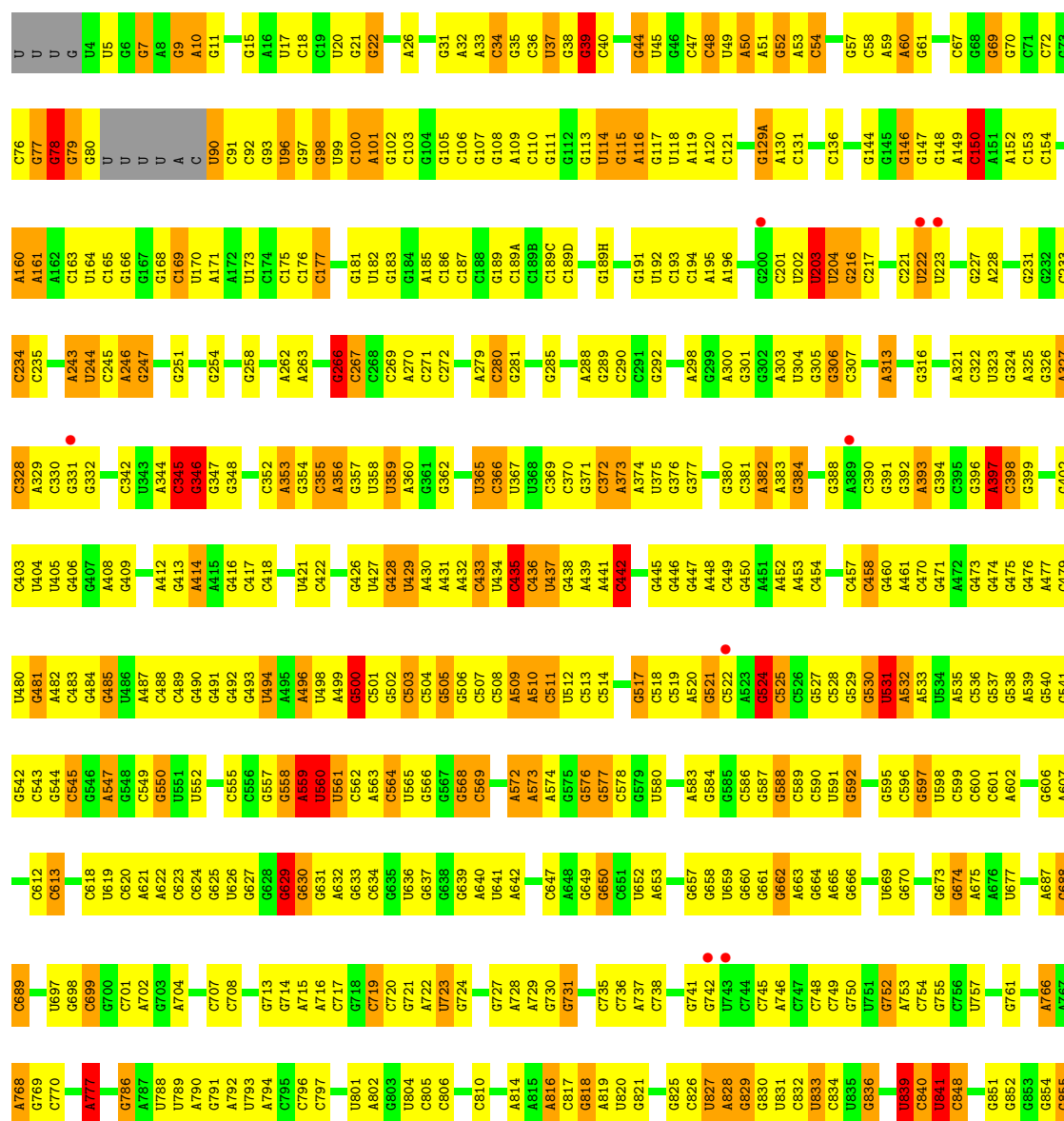


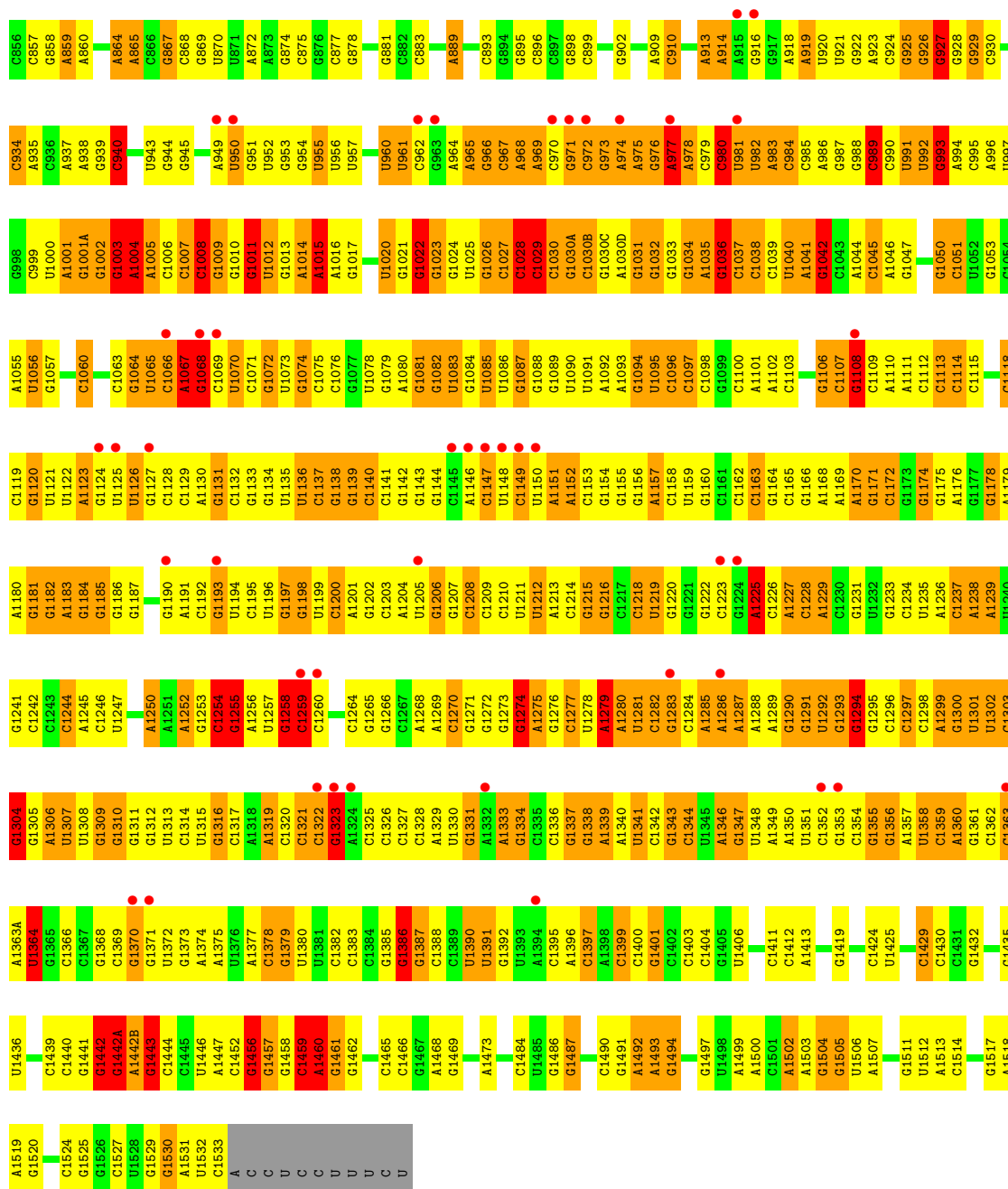
### 3 Residue-property plots

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.

#### • Molecule 1: 16S ribosomal RNA

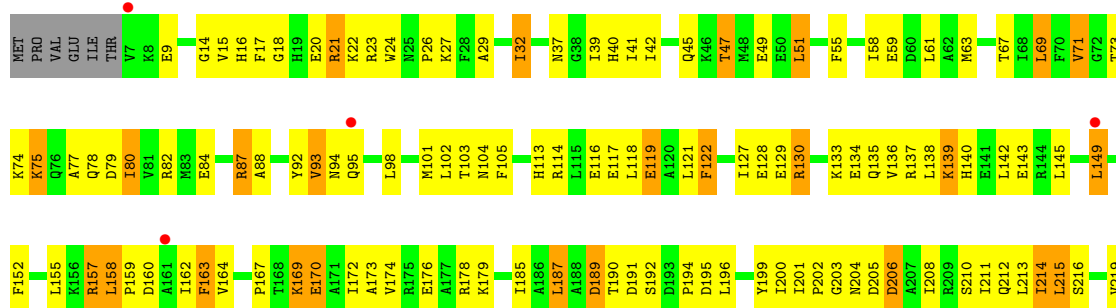
Chain A: 

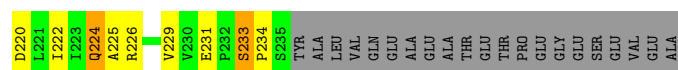




• Molecule 2: 30S ribosomal protein S2

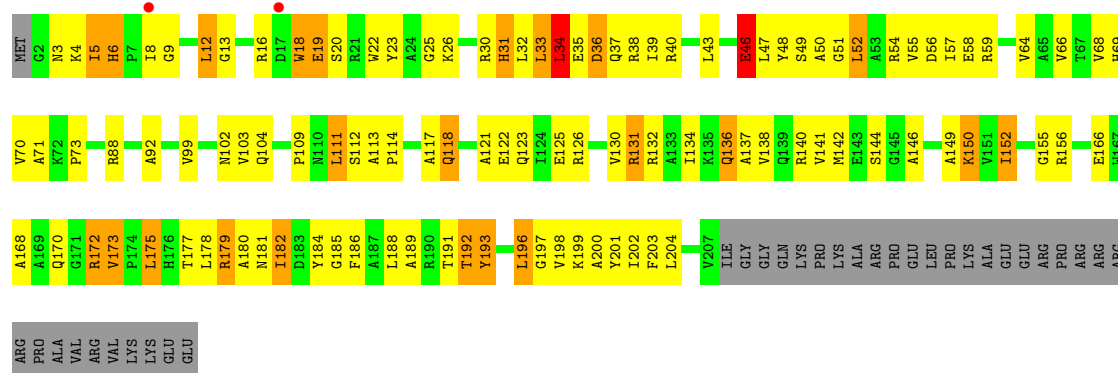
Chain B:





• Molecule 3: 30S ribosomal protein S3

Chain C:



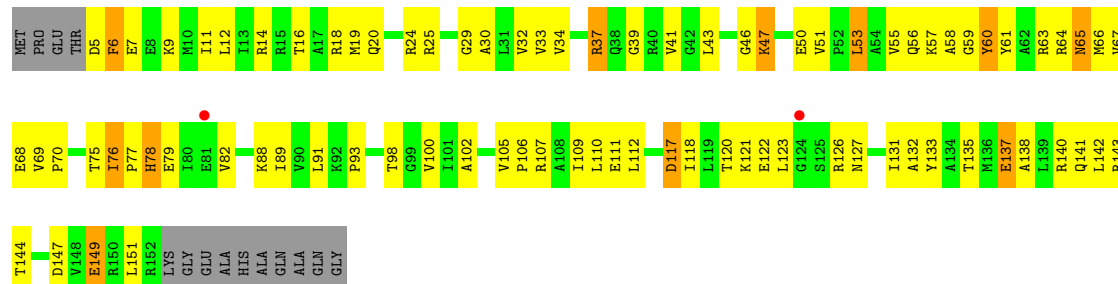
• Molecule 4: 30S ribosomal protein S4

Chain D:



• Molecule 5: 30S ribosomal protein S5

Chain E:



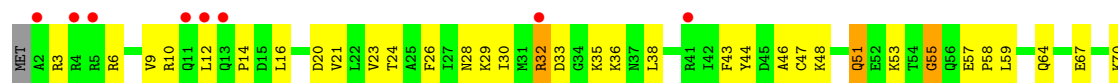
• Molecule 6: 30S ribosomal protein S6

Chain F:



• Molecule 7: 30S ribosomal protein S7

Chain G:



- Molecule 8: 30S ribosomal protein S8

Chain H:



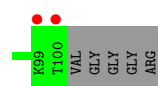
- Molecule 9: 30S ribosomal protein S9

Chain I:



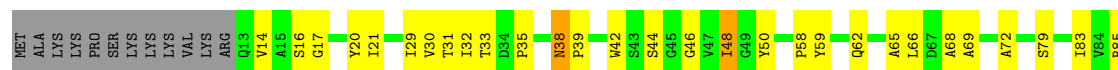
- Molecule 10: 30S ribosomal protein S10

Chain J:



- Molecule 11: 30S ribosomal protein S11

Chain K:



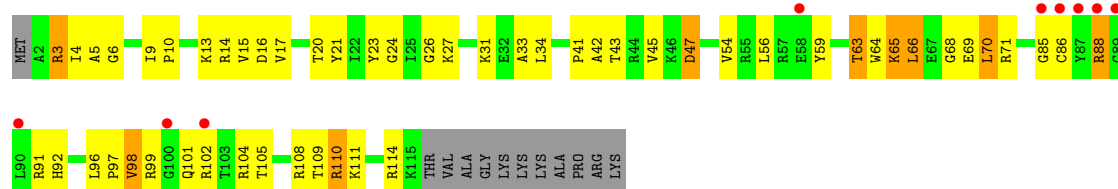
- Molecule 12: 30S ribosomal protein S12

Chain L:



- Molecule 13: 30S ribosomal protein S13

Chain M:



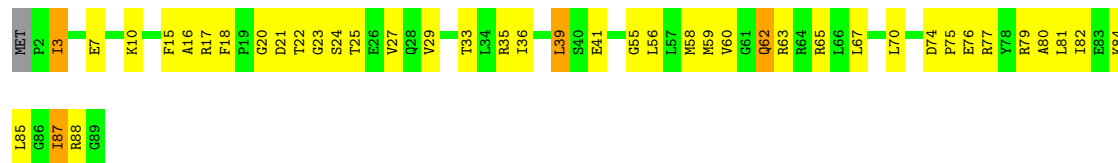
- Molecule 14: 30S ribosomal protein S14

Chain N:



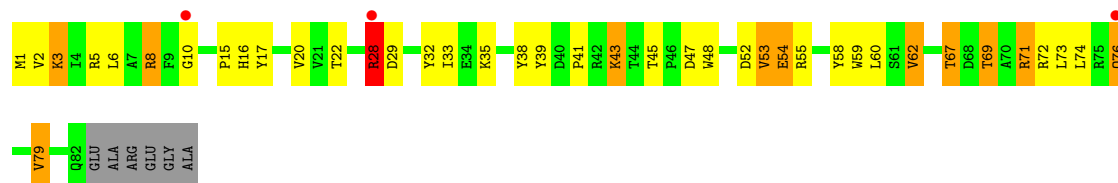
- Molecule 15: 30S ribosomal protein S15

Chain O:



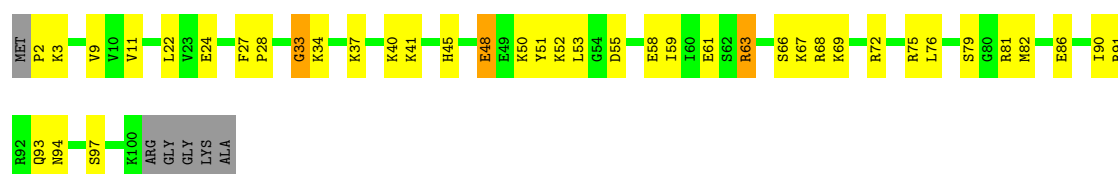
- Molecule 16: 30S ribosomal protein S16

Chain P:

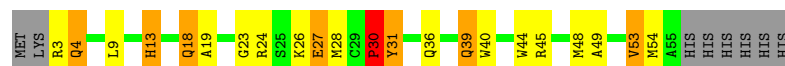
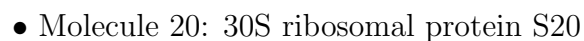
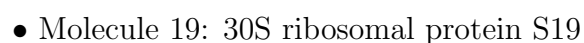


- Molecule 17: 30S ribosomal protein S17

Chain Q:



- Chain R:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.24Å 451.44Å 621.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 3.00 49.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.75-3.00) 98.0 (49.75-3.00)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.218 , 0.254 0.512 , 0.514	Depositor DCC
$R_{free}$ test set	57194 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 74.2	EDS
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 1142037 reflections	Xtriage
$F_o, F_c$ correlation	0.49	EDS
Total number of atoms	50378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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	0.91	21/36123 (0.1%)	1.38	452/56379 (0.8%)
2	B	0.61	0/1809	0.73	1/2450 (0.0%)
3	C	0.68	0/1474	0.79	2/2003 (0.1%)
4	D	0.64	2/1556 (0.1%)	0.74	2/2113 (0.1%)
5	E	0.58	0/1121	0.78	1/1517 (0.1%)
6	F	0.54	0/790	0.70	0/1077
7	G	0.72	0/1183	0.77	0/1599
8	H	0.50	0/1065	0.67	0/1445
9	I	0.74	0/867	0.84	1/1180 (0.1%)
10	J	0.75	0/676	0.88	2/924 (0.2%)
11	K	0.53	0/843	0.69	0/1144
12	L	0.54	0/921	0.73	0/1247
13	M	0.72	0/814	0.83	0/1107
14	N	0.66	0/487	0.71	1/649 (0.2%)
15	O	0.52	0/735	0.72	0/981
16	P	0.54	0/667	0.84	1/905 (0.1%)
17	Q	0.57	0/836	0.72	0/1117
18	R	0.56	0/519	0.79	0/699
19	S	0.69	0/574	0.81	0/781
20	T	0.52	0/715	0.77	0/947
21	U	0.73	0/203	0.68	0/266
22	V	0.65	0/360	0.85	1/492 (0.2%)
All	All	0.82	23/54338 (0.0%)	1.22	464/81022 (0.6%)

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	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
5	E	0	1
7	G	0	1
9	I	0	1
12	L	0	1
13	M	0	1
17	Q	0	1
20	T	0	1
22	V	0	3
All	All	0	15

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1459	C	N1-C2	17.17	1.57	1.40
1	A	1442(A)	G	N9-C4	15.91	1.50	1.38
1	A	90	U	C4-O4	13.40	1.34	1.23
1	A	1442(A)	G	C2-N3	11.63	1.42	1.32
1	A	1459	C	C1'-N1	10.41	1.64	1.48
4	D	9	CYS	CB-SG	9.32	1.98	1.82
1	A	1442(A)	G	N3-C4	9.30	1.42	1.35
1	A	1459	C	C2-N3	8.70	1.42	1.35
1	A	69	G	O3'-P	-8.45	1.51	1.61
1	A	1123	A	N9-C4	7.03	1.42	1.37
1	A	1087	G	N9-C4	7.01	1.43	1.38
1	A	1031	G	N3-C4	7.00	1.40	1.35
1	A	977	A	N9-C4	5.82	1.41	1.37
4	D	12	CYS	CB-SG	5.75	1.92	1.82
1	A	1459	C	P-O5'	5.50	1.65	1.59
1	A	1170	A	N9-C4	5.44	1.41	1.37
1	A	346	G	N7-C5	-5.37	1.36	1.39
1	A	1093	A	N9-C4	5.35	1.41	1.37
1	A	1459	C	C2-O2	5.28	1.29	1.24
1	A	346	G	C6-N1	-5.25	1.35	1.39
1	A	839	U	N1-C2	5.16	1.43	1.38
1	A	928	G	C6-N1	5.09	1.43	1.39
1	A	1191	A	N9-C4	5.03	1.40	1.37

All (464) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1442(A)	G	N3-C4-C5	-27.29	114.95	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1459	C	N3-C2-O2	-27.00	103.00	121.90
1	A	1459	C	C6-N1-C2	-26.34	109.77	120.30
1	A	1442(A)	G	N3-C4-N9	23.46	140.08	126.00
1	A	1459	C	N1-C2-O2	21.61	131.87	118.90
1	A	1030	C	N1-C2-O2	21.33	131.70	118.90
1	A	1442(A)	G	C6-N1-C2	-18.82	113.81	125.10
1	A	1442(A)	G	C4-N9-C1'	18.22	150.19	126.50
1	A	1442(A)	G	C5-C6-N1	17.80	120.40	111.50
1	A	1459	C	C2-N1-C1'	17.05	137.55	118.80
1	A	1442(A)	G	C2-N3-C4	15.44	119.62	111.90
1	A	1442(A)	G	C8-N9-C1'	-14.54	108.10	127.00
1	A	1442(A)	G	C8-N9-C4	-14.43	100.63	106.40
1	A	1031	G	N3-C2-N2	14.29	129.90	119.90
1	A	1003	G	C5-C6-O6	13.36	136.62	128.60
1	A	1442(A)	G	C5-C6-O6	-13.09	120.75	128.60
1	A	1030	C	N3-C2-O2	-12.56	113.11	121.90
1	A	90	U	N3-C4-C5	12.26	121.95	114.60
1	A	1031	G	N9-C4-C5	-12.12	100.55	105.40
1	A	346	G	C4-N9-C1'	11.88	141.95	126.50
1	A	1003	G	N1-C6-O6	-11.74	112.86	119.90
1	A	1442(A)	G	C6-C5-N7	-11.09	123.75	130.40
1	A	1484	C	C6-N1-C2	10.82	124.63	120.30
1	A	346	G	C8-N9-C1'	-10.73	113.06	127.00
1	A	1087	G	N3-C4-C5	-10.58	123.31	128.60
1	A	1459	C	C5-C6-N1	10.54	126.27	121.00
1	A	1442(A)	G	N1-C2-N2	-10.40	106.84	116.20
1	A	1442(A)	G	N7-C8-N9	10.05	118.12	113.10
1	A	90	U	C2-N3-C4	-10.00	121.00	127.00
1	A	1031	G	C4-C5-N7	9.91	114.77	110.80
1	A	1459	C	C2-N3-C4	-9.82	114.99	119.90
1	A	1395	C	C6-N1-C2	-9.70	116.42	120.30
1	A	1030	C	C2-N3-C4	9.64	124.72	119.90
1	A	1028	C	N1-C2-O2	9.49	124.59	118.90
1	A	1395	C	N3-C4-C5	-9.44	118.12	121.90
1	A	1442(A)	G	C4-C5-C6	9.34	124.40	118.80
1	A	1442(A)	G	N3-C2-N2	9.26	126.38	119.90
1	A	1391	U	N3-C2-O2	-9.10	115.83	122.20
1	A	1274	G	C4-N9-C1'	9.09	138.31	126.50
1	A	1378	C	C6-N1-C2	-9.00	116.70	120.30
1	A	1242	C	C5-C6-N1	8.90	125.45	121.00
1	A	1442(A)	G	O4'-C1'-N9	8.87	115.30	108.20
1	A	1456	G	C4-N9-C1'	8.85	138.00	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	839	U	N1-C2-O2	8.80	128.96	122.80
1	A	1460	A	N1-C6-N6	-8.79	113.33	118.60
1	A	346	G	N3-C4-C5	-8.77	124.22	128.60
1	A	1037	C	C2-N3-C4	8.66	124.23	119.90
1	A	1087	G	N3-C4-N9	8.63	131.18	126.00
1	A	1031	G	C6-N1-C2	8.62	130.27	125.10
1	A	1037	C	N3-C4-C5	-8.61	118.46	121.90
1	A	1274	G	N7-C8-N9	8.52	117.36	113.10
1	A	1459	C	N1-C2-N3	8.47	125.13	119.20
1	A	1283	G	N3-C2-N2	-8.47	113.97	119.90
1	A	1391	U	C5-C4-O4	8.46	130.98	125.90
1	A	150	C	C5-C6-N1	8.42	125.21	121.00
1	A	1274	G	C6-C5-N7	-8.41	125.35	130.40
1	A	90	U	C5-C4-O4	-8.40	120.86	125.90
1	A	1277	C	C6-N1-C2	-8.38	116.95	120.30
1	A	1031	G	N3-C4-N9	8.23	130.94	126.00
1	A	399	G	N1-C6-O6	8.17	124.80	119.90
1	A	955	U	C2-N3-C4	8.15	131.89	127.00
1	A	346	G	N3-C4-N9	8.09	130.85	126.00
1	A	1036	G	C4-N9-C1'	8.08	137.00	126.50
1	A	1391	U	N1-C2-O2	8.05	128.44	122.80
1	A	910	C	C6-N1-C2	7.99	123.49	120.30
1	A	1456	G	C8-N9-C4	-7.97	103.21	106.40
1	A	572	A	C8-N9-C4	7.90	108.96	105.80
1	A	1502	A	C5-N7-C8	-7.88	99.96	103.90
1	A	898	G	C8-N9-C4	7.88	109.55	106.40
1	A	1456	G	N7-C8-N9	7.88	117.04	113.10
1	A	1205	U	C6-N1-C2	-7.80	116.32	121.00
1	A	1387	G	C8-N9-C4	7.77	109.51	106.40
1	A	1015	A	C8-N9-C4	-7.73	102.71	105.80
1	A	346	G	N1-C2-N2	-7.72	109.25	116.20
1	A	1274	G	C8-N9-C4	-7.65	103.34	106.40
1	A	1126	U	C5-C6-N1	7.61	126.50	122.70
1	A	1254	C	C6-N1-C2	-7.59	117.27	120.30
1	A	1216	G	N3-C4-C5	7.57	132.38	128.60
1	A	697	U	C5-C6-N1	-7.56	118.92	122.70
1	A	529	G	N1-C6-O6	7.55	124.43	119.90
1	A	1003	G	N3-C4-N9	-7.54	121.48	126.00
1	A	839	U	C2-N1-C1'	7.50	126.70	117.70
1	A	1030(B)	C	N3-C2-O2	-7.48	116.66	121.90
1	A	44	G	N1-C6-O6	7.48	124.39	119.90
1	A	1015	A	N7-C8-N9	7.47	117.53	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	754	C	N1-C2-O2	7.42	123.36	118.90
1	A	1030(B)	C	N1-C2-O2	7.42	123.35	118.90
1	A	995	C	C6-N1-C2	-7.38	117.35	120.30
1	A	1277	C	N1-C2-O2	7.36	123.31	118.90
1	A	1030(B)	C	C6-N1-C2	-7.34	117.36	120.30
1	A	997	U	C5-C4-O4	7.32	130.29	125.90
1	A	345	C	C2-N1-C1'	7.32	126.85	118.80
1	A	993	G	C2-N3-C4	7.30	115.55	111.90
1	A	503	C	C6-N1-C2	-7.30	117.38	120.30
1	A	365	U	C2-N1-C1'	-7.29	108.95	117.70
1	A	766	A	C8-N9-C4	7.28	108.71	105.80
1	A	1031	G	N1-C2-N3	-7.28	119.53	123.90
1	A	1006	C	C6-N1-C2	-7.28	117.39	120.30
1	A	1011	G	N7-C8-N9	7.27	116.73	113.10
1	A	1519	A	N9-C4-C5	7.24	108.69	105.80
1	A	39	G	C6-N1-C2	-7.22	120.77	125.10
1	A	1283	G	N3-C4-N9	-7.17	121.70	126.00
1	A	1216	G	C4-N9-C1'	-7.12	117.24	126.50
1	A	1003	G	N9-C4-C5	7.10	108.24	105.40
1	A	754	C	N3-C2-O2	-7.08	116.94	121.90
1	A	1036	G	C8-N9-C1'	-7.08	117.80	127.00
1	A	995	C	N1-C2-O2	7.07	123.14	118.90
1	A	1277	C	C2-N3-C4	7.06	123.43	119.90
1	A	839	U	N3-C2-O2	-7.06	117.26	122.20
1	A	1216	G	N3-C4-N9	-7.04	121.78	126.00
1	A	1069	C	C6-N1-C2	-7.03	117.49	120.30
1	A	1456	G	C6-C5-N7	-7.03	126.18	130.40
1	A	1502	A	C4-C5-N7	6.99	114.19	110.70
1	A	1459	C	C4-C5-C6	6.98	120.89	117.40
1	A	1277	C	C5-C6-N1	6.98	124.49	121.00
1	A	1008	C	N1-C2-O2	6.95	123.07	118.90
1	A	346	G	C4-C5-C6	6.92	122.95	118.80
1	A	1044	A	C5-C6-N6	6.90	129.22	123.70
1	A	365	U	C5-C6-N1	-6.89	119.25	122.70
1	A	1443	G	C5-C6-N1	6.89	114.94	111.50
1	A	1087	G	C4-N9-C1'	6.85	135.41	126.50
1	A	1258	G	C2-N3-C4	6.83	115.31	111.90
1	A	1368	G	N1-C6-O6	6.81	123.99	119.90
1	A	1290	G	C5-C6-O6	6.80	132.68	128.60
1	A	1002	G	C8-N9-C4	-6.78	103.69	106.40
1	A	1459	C	C6-N1-C1'	-6.78	112.67	120.80
1	A	117	G	C6-C5-N7	-6.75	126.35	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1344	C	C6-N1-C2	-6.73	117.61	120.30
1	A	1037	C	C5-C4-N4	6.73	124.91	120.20
1	A	1242	C	C6-N1-C2	-6.71	117.62	120.30
1	A	403	C	C2-N3-C4	-6.70	116.55	119.90
1	A	1026	G	C4-N9-C1'	6.70	135.22	126.50
1	A	1274	G	C8-N9-C1'	-6.70	118.28	127.00
1	A	757	U	C5-C6-N1	-6.70	119.35	122.70
1	A	1195	C	C6-N1-C2	-6.68	117.63	120.30
1	A	754	C	C2-N1-C1'	6.67	126.14	118.80
1	A	1151	A	N1-C6-N6	-6.66	114.60	118.60
1	A	768	A	C8-N9-C4	6.65	108.46	105.80
1	A	898	G	N9-C4-C5	-6.64	102.74	105.40
1	A	1038	C	C2-N3-C4	6.64	123.22	119.90
1	A	357	G	C2-N3-C4	6.63	115.22	111.90
1	A	1242	C	N3-C4-N4	6.62	122.63	118.00
1	A	1524	C	C6-N1-C2	6.57	122.93	120.30
1	A	346	G	C6-C5-N7	-6.56	126.47	130.40
1	A	1460	A	C5-N7-C8	6.55	107.17	103.90
1	A	1028	C	C2-N3-C4	6.53	123.17	119.90
1	A	524	G	C8-N9-C4	-6.53	103.79	106.40
1	A	699	C	C6-N1-C2	-6.52	117.69	120.30
1	A	1000	U	C2-N3-C4	6.51	130.91	127.00
1	A	1502	A	N1-C6-N6	6.48	122.49	118.60
1	A	950	U	N1-C2-O2	6.46	127.32	122.80
1	A	697	U	C2-N1-C1'	-6.45	109.96	117.70
1	A	1218	C	N3-C2-O2	-6.45	117.39	121.90
1	A	169	C	C6-N1-C2	-6.43	117.73	120.30
1	A	1432	G	N3-C4-N9	-6.42	122.15	126.00
1	A	117	G	N1-C6-O6	6.42	123.75	119.90
1	A	52	G	N1-C6-O6	-6.41	116.05	119.90
1	A	1056	U	N1-C2-O2	6.40	127.28	122.80
1	A	1307	U	C5-C6-N1	6.39	125.90	122.70
1	A	1067	A	C8-N9-C4	-6.37	103.25	105.80
1	A	117	G	C5-C6-O6	-6.36	124.78	128.60
1	A	355	C	C6-N1-C2	-6.34	117.76	120.30
1	A	1003	G	C6-C5-N7	6.33	134.20	130.40
1	A	1460	A	C6-C5-N7	6.33	136.73	132.30
1	A	1456	G	C8-N9-C1'	-6.32	118.78	127.00
1	A	777	A	C8-N9-C4	-6.31	103.28	105.80
1	A	1283	G	N9-C4-C5	6.28	107.91	105.40
1	A	1279	A	N7-C8-N9	6.27	116.94	113.80
1	A	1387	G	N9-C4-C5	-6.27	102.89	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1029	C	C6-N1-C2	-6.27	117.79	120.30
1	A	997	U	C2-N3-C4	6.27	130.76	127.00
1	A	1519	A	C8-N9-C4	-6.27	103.29	105.80
1	A	1031	G	N1-C2-N2	-6.27	110.56	116.20
1	A	372	C	N1-C2-O2	6.26	122.65	118.90
1	A	1151	A	C5-C6-N6	6.24	128.69	123.70
1	A	357	G	C5-C6-N1	6.23	114.61	111.50
1	A	397	A	C8-N9-C4	-6.23	103.31	105.80
1	A	53	A	N1-C6-N6	-6.20	114.88	118.60
1	A	150	C	C6-N1-C2	-6.20	117.82	120.30
1	A	1068	G	C8-N9-C4	-6.16	103.94	106.40
1	A	52	G	C5-C6-O6	6.16	132.29	128.60
1	A	1056	U	C5-C4-O4	6.15	129.59	125.90
1	A	995	C	C2-N1-C1'	6.14	125.56	118.80
1	A	1276	G	N3-C4-N9	6.14	129.68	126.00
1	A	1364	U	N3-C2-O2	-6.14	117.90	122.20
1	A	1277	C	N3-C4-C5	-6.13	119.45	121.90
1	A	766	A	N1-C6-N6	6.11	122.27	118.60
1	A	1044	A	N1-C6-N6	-6.11	114.94	118.60
1	A	895	G	N1-C6-O6	6.09	123.55	119.90
1	A	1456	G	N3-C4-C5	-6.09	125.56	128.60
1	A	500	G	N1-C6-O6	-6.07	116.26	119.90
1	A	1242	C	C2-N3-C4	6.06	122.93	119.90
1	A	346	G	N3-C2-N2	6.06	124.14	119.90
1	A	1030	C	C2-N1-C1'	6.06	125.47	118.80
1	A	1484	C	N3-C4-C5	6.04	124.32	121.90
1	A	766	A	N9-C4-C5	-6.03	103.39	105.80
1	A	1456	G	N3-C4-N9	6.03	129.62	126.00
1	A	1032	G	C5-C6-N1	-6.03	108.49	111.50
1	A	1121	U	C5-C6-N1	6.02	125.71	122.70
1	A	1395	C	C5-C6-N1	6.02	124.01	121.00
1	A	995	C	C5-C6-N1	6.01	124.01	121.00
1	A	37	U	N3-C2-O2	-6.01	118.00	122.20
1	A	1442(B)	A	N1-C2-N3	5.98	132.29	129.30
1	A	397	A	N9-C4-C5	5.98	108.19	105.80
1	A	896	C	C6-N1-C2	5.98	122.69	120.30
10	J	90	LEU	C-N-CD	-5.98	107.45	120.60
1	A	357	G	N1-C6-O6	-5.98	116.31	119.90
4	D	12	CYS	CA-CB-SG	5.97	124.75	114.00
1	A	1038	C	C6-N1-C2	-5.97	117.91	120.30
1	A	569	C	C6-N1-C2	-5.96	117.91	120.30
1	A	1036	G	N3-C4-N9	5.94	129.56	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	A	N7-C8-N9	-5.93	110.83	113.80
1	A	993	G	N3-C4-N9	5.92	129.55	126.00
1	A	1123	A	C8-N9-C4	-5.92	103.43	105.80
1	A	1326	C	C6-N1-C2	5.91	122.66	120.30
1	A	896	C	N3-C4-C5	5.91	124.26	121.90
1	A	1041	A	C5-C6-N6	5.90	128.42	123.70
1	A	345	C	C6-N1-C1'	-5.89	113.73	120.80
1	A	1519	A	N1-C6-N6	-5.89	115.06	118.60
1	A	525	C	C5-C6-N1	5.87	123.94	121.00
1	A	1216	G	C8-N9-C1'	5.87	134.62	127.00
1	A	1294	G	C8-N9-C1'	5.85	134.61	127.00
1	A	39	G	N3-C4-C5	-5.85	125.67	128.60
1	A	357	G	C6-N1-C2	-5.85	121.59	125.10
1	A	1093	A	C8-N9-C4	-5.83	103.47	105.80
1	A	1012	U	C6-N1-C2	-5.82	117.51	121.00
1	A	1051	C	C5-C6-N1	5.82	123.91	121.00
3	C	196	LEU	CA-CB-CG	5.82	128.68	115.30
14	N	44	LEU	CA-CB-CG	5.82	128.68	115.30
1	A	496	A	N1-C6-N6	-5.81	115.11	118.60
1	A	766	A	C5-C6-N6	-5.81	119.05	123.70
1	A	1429	C	C6-N1-C2	5.81	122.63	120.30
1	A	977	A	C2-N3-C4	5.81	113.50	110.60
1	A	54	C	C2-N3-C4	-5.81	117.00	119.90
1	A	770	C	N3-C4-C5	-5.80	119.58	121.90
1	A	235	C	N1-C2-O2	5.80	122.38	118.90
1	A	1518	A	C8-N9-C4	-5.80	103.48	105.80
1	A	117	G	N3-C4-N9	5.79	129.48	126.00
1	A	1502	A	N7-C8-N9	5.79	116.70	113.80
1	A	867	G	N3-C4-C5	-5.79	125.71	128.60
1	A	1460	A	N7-C8-N9	-5.79	110.91	113.80
1	A	973	G	C5-C6-O6	-5.78	125.13	128.60
1	A	1197	G	N3-C4-C5	-5.78	125.71	128.60
1	A	1283	G	N1-C2-N2	5.77	121.40	116.20
1	A	1356	G	C8-N9-C4	-5.76	104.10	106.40
1	A	359	U	C2-N3-C4	-5.76	123.55	127.00
1	A	1237	C	C6-N1-C2	-5.76	118.00	120.30
1	A	1044	A	C6-N1-C2	5.75	122.05	118.60
1	A	1527	C	C6-N1-C2	5.75	122.60	120.30
1	A	357	G	N3-C4-C5	-5.75	125.72	128.60
1	A	1397	C	C2-N1-C1'	5.74	125.11	118.80
1	A	910	C	N3-C4-C5	5.74	124.20	121.90
1	A	1030(B)	C	C2-N1-C1'	5.74	125.11	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	A	C8-N9-C4	-5.72	103.51	105.80
1	A	1030	C	N1-C2-N3	-5.72	115.20	119.20
1	A	1502	A	C6-C5-N7	-5.72	128.30	132.30
1	A	689	C	C6-N1-C2	-5.71	118.01	120.30
1	A	1294	G	C4-N9-C1'	-5.71	119.07	126.50
1	A	1031	G	C8-N9-C4	5.70	108.68	106.40
1	A	442	C	C6-N1-C2	-5.69	118.02	120.30
1	A	1037	C	C6-N1-C2	-5.69	118.02	120.30
1	A	1123	A	C6-N1-C2	-5.68	115.19	118.60
1	A	1519	A	C4-C5-N7	-5.67	107.86	110.70
1	A	1259	C	C5-C6-N1	5.67	123.83	121.00
1	A	53	A	C5-C6-N6	5.66	128.23	123.70
1	A	1036	G	C6-C5-N7	-5.66	127.00	130.40
1	A	852	G	N3-C4-N9	-5.66	122.61	126.00
1	A	1254	C	C5-C6-N1	5.66	123.83	121.00
1	A	989	C	C2-N3-C4	5.65	122.73	119.90
1	A	1029	C	N3-C2-O2	-5.65	117.94	121.90
1	A	841	U	C6-N1-C2	-5.65	117.61	121.00
1	A	1074	G	C5-C6-N1	-5.65	108.67	111.50
1	A	90	U	N1-C2-N3	5.64	118.29	114.90
1	A	1022	G	C5-C6-O6	-5.63	125.22	128.60
1	A	1003	G	C4-C5-N7	-5.63	108.55	110.80
1	A	1216	G	C6-N1-C2	5.62	128.47	125.10
1	A	1041	A	C6-N1-C2	5.62	121.97	118.60
1	A	981	U	C5-C6-N1	5.62	125.51	122.70
1	A	1032	G	C6-N1-C2	5.61	128.47	125.10
1	A	1197	G	C4-N9-C1'	5.61	133.79	126.50
1	A	1002	G	N7-C8-N9	5.61	115.90	113.10
1	A	572	A	C4-N9-C1'	-5.60	116.22	126.30
1	A	489	C	C5-C6-N1	5.60	123.80	121.00
1	A	1197	G	N3-C4-N9	5.59	129.35	126.00
1	A	1006	C	N3-C4-C5	-5.58	119.67	121.90
1	A	1391	U	N3-C4-O4	-5.57	115.50	119.40
1	A	1439	C	N1-C2-O2	-5.56	115.56	118.90
1	A	1097	C	N1-C2-O2	5.56	122.24	118.90
1	A	530	G	C4-N9-C1'	5.56	133.73	126.50
1	A	1032	G	N3-C4-N9	-5.56	122.66	126.00
1	A	1279	A	C8-N9-C4	-5.56	103.58	105.80
1	A	1258	G	N1-C2-N3	-5.55	120.57	123.90
1	A	1277	C	C2-N1-C1'	5.54	124.90	118.80
1	A	674	G	C4-C5-N7	5.54	113.01	110.80
1	A	1255	G	N1-C6-O6	5.53	123.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	927	G	C5-C6-O6	5.53	131.92	128.60
1	A	1326	C	C2-N1-C1'	-5.52	112.73	118.80
1	A	78	G	N1-C6-O6	5.51	123.21	119.90
1	A	1038	C	C5-C6-N1	5.50	123.75	121.00
1	A	1087	G	C2-N3-C4	5.50	114.65	111.90
1	A	397	A	N1-C2-N3	5.49	132.05	129.30
1	A	754	C	C6-N1-C2	-5.49	118.10	120.30
1	A	1218	C	N1-C2-O2	5.49	122.19	118.90
1	A	1459	C	O4'-C1'-N1	5.49	112.59	108.20
1	A	39	G	N1-C6-O6	-5.49	116.61	119.90
1	A	1499	A	N1-C6-N6	5.49	121.89	118.60
1	A	929	G	C4-C5-N7	-5.48	108.61	110.80
1	A	494	U	C5-C6-N1	5.48	125.44	122.70
1	A	993	G	N3-C4-C5	-5.48	125.86	128.60
1	A	1060	C	C6-N1-C2	-5.47	118.11	120.30
1	A	955	U	C5-C6-N1	5.47	125.43	122.70
1	A	1056	U	C2-N3-C4	5.47	130.28	127.00
16	P	28	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	403	C	N3-C2-O2	-5.46	118.08	121.90
1	A	810	C	N3-C4-C5	5.46	124.08	121.90
1	A	402	G	N1-C6-O6	-5.46	116.62	119.90
1	A	865	A	N7-C8-N9	5.46	116.53	113.80
1	A	1015	A	N1-C2-N3	5.46	132.03	129.30
1	A	1163	C	C6-N1-C2	-5.46	118.12	120.30
1	A	1005	A	N7-C8-N9	5.46	116.53	113.80
1	A	506	G	C8-N9-C4	-5.45	104.22	106.40
1	A	893	C	N1-C2-O2	5.45	122.17	118.90
1	A	1026	G	C8-N9-C4	-5.45	104.22	106.40
1	A	1067	A	N7-C8-N9	5.45	116.53	113.80
1	A	345	C	C5-C6-N1	5.45	123.72	121.00
1	A	1194	U	N3-C2-O2	-5.45	118.39	122.20
1	A	530	G	C8-N9-C1'	-5.44	119.92	127.00
1	A	1519	A	N1-C2-N3	5.44	132.02	129.30
9	I	24	GLY	N-CA-C	5.44	126.70	113.10
1	A	1112	C	C6-N1-C2	-5.44	118.12	120.30
1	A	381	C	C6-N1-C2	-5.43	118.13	120.30
1	A	1108	G	C4-N9-C1'	5.43	133.56	126.50
1	A	1158	C	N1-C2-O2	5.42	122.15	118.90
1	A	1527	C	N3-C4-C5	5.42	124.07	121.90
1	A	1216	G	C6-C5-N7	5.42	133.65	130.40
1	A	435	C	C5-C6-N1	5.42	123.71	121.00
1	A	356	A	C2-N3-C4	5.41	113.31	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1014	A	C8-N9-C4	-5.41	103.64	105.80
1	A	1012	U	C5-C6-N1	5.41	125.41	122.70
1	A	1030(D)	A	C8-N9-C4	-5.41	103.64	105.80
1	A	1096	C	C6-N1-C2	-5.39	118.14	120.30
1	A	1378	C	N3-C2-O2	-5.37	118.14	121.90
1	A	940	C	N1-C2-O2	5.37	122.12	118.90
1	A	899	C	C6-N1-C2	5.37	122.45	120.30
1	A	919	A	C2-N3-C4	5.37	113.28	110.60
1	A	1274	G	C4-C5-C6	5.37	122.02	118.80
1	A	1440	C	C6-N1-C2	5.36	122.44	120.30
1	A	576	G	C4-N9-C1'	5.35	133.46	126.50
1	A	1087	G	C8-N9-C1'	-5.35	120.05	127.00
1	A	1149	C	C6-N1-C2	-5.35	118.16	120.30
1	A	234	C	N1-C2-O2	5.35	122.11	118.90
1	A	1006	C	C2-N3-C4	5.35	122.57	119.90
1	A	177	C	C6-N1-C2	-5.34	118.16	120.30
1	A	1274	G	N1-C6-O6	5.34	123.10	119.90
1	A	1519	A	C5-C6-N6	5.34	127.97	123.70
1	A	1323	G	N3-C4-N9	5.34	129.20	126.00
1	A	1462	G	N3-C2-N2	-5.33	116.17	119.90
2	B	169	LYS	N-CA-C	-5.33	96.60	111.00
1	A	1041	A	N1-C6-N6	-5.33	115.40	118.60
1	A	1083	U	N1-C2-O2	-5.33	119.07	122.80
1	A	1390	U	N1-C2-O2	-5.33	119.07	122.80
1	A	246	A	C8-N9-C4	5.33	107.93	105.80
1	A	365	U	C6-N1-C1'	5.33	128.66	121.20
1	A	1038	C	N3-C4-C5	-5.33	119.77	121.90
1	A	1442	G	N3-C4-N9	5.31	129.19	126.00
1	A	393	A	C8-N9-C4	-5.31	103.68	105.80
1	A	893	C	C6-N1-C2	5.31	122.42	120.30
1	A	980	C	N1-C2-O2	5.31	122.09	118.90
5	E	65	ASN	N-CA-C	-5.31	96.67	111.00
10	J	16	LEU	CA-CB-CG	5.31	127.50	115.30
1	A	500	G	C5-C6-O6	5.30	131.78	128.60
1	A	1149	C	C5-C6-N1	5.30	123.65	121.00
1	A	1030	C	C6-N1-C1'	-5.30	114.44	120.80
1	A	1123	A	N3-C4-C5	-5.29	123.09	126.80
1	A	1195	C	C5-C6-N1	5.29	123.65	121.00
1	A	945	G	C8-N9-C4	5.29	108.52	106.40
1	A	697	U	C6-N1-C2	5.29	124.17	121.00
1	A	1386	G	C6-C5-N7	5.29	133.57	130.40
1	A	105	G	C8-N9-C4	-5.29	104.28	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	9	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	358	U	C5-C4-O4	5.28	129.07	125.90
1	A	839	U	C6-N1-C1'	-5.27	113.82	121.20
1	A	1304	G	C2-N3-C4	5.27	114.53	111.90
1	A	1460	A	C5-C6-N6	5.26	127.91	123.70
1	A	1432	G	N3-C4-C5	5.25	131.22	128.60
1	A	674	G	C5-C6-O6	-5.25	125.45	128.60
1	A	727	G	N1-C6-O6	-5.24	116.76	119.90
1	A	266	G	N3-C4-N9	-5.24	122.86	126.00
1	A	629	G	C8-N9-C4	-5.24	104.31	106.40
1	A	865	A	C8-N9-C4	-5.23	103.71	105.80
1	A	1274	G	N3-C4-N9	5.23	129.14	126.00
1	A	292	G	C8-N9-C4	-5.23	104.31	106.40
1	A	1334	G	N3-C4-N9	5.22	129.13	126.00
1	A	1194	U	C6-N1-C2	-5.21	117.87	121.00
1	A	980	C	C6-N1-C2	-5.21	118.22	120.30
1	A	1042	G	N3-C4-N9	-5.20	122.88	126.00
1	A	114	U	N3-C2-O2	-5.20	118.56	122.20
1	A	1395	C	C2-N3-C4	5.19	122.49	119.90
1	A	578	C	C6-N1-C2	-5.17	118.23	120.30
1	A	1083	U	C4-C5-C6	5.17	122.80	119.70
3	C	34	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	967	C	C5-C6-N1	5.16	123.58	121.00
1	A	517	G	N1-C6-O6	-5.16	116.80	119.90
1	A	1225	A	C6-N1-C2	5.16	121.69	118.60
1	A	34	C	C6-N1-C2	5.15	122.36	120.30
1	A	576	G	C8-N9-C1'	-5.15	120.30	127.00
1	A	719	C	C6-N1-C2	-5.15	118.24	120.30
1	A	923	A	N1-C2-N3	5.15	131.88	129.30
1	A	1219	U	C5-C4-O4	-5.14	122.81	125.90
1	A	1343	G	N3-C4-N9	5.14	129.09	126.00
1	A	1378	C	C2-N1-C1'	5.14	124.46	118.80
4	D	9	CYS	CA-CB-SG	5.14	123.26	114.00
1	A	290	C	N1-C2-O2	-5.14	115.82	118.90
1	A	973	G	N1-C6-O6	5.14	122.98	119.90
1	A	1443	G	C4-C5-N7	5.14	112.86	110.80
1	A	345	C	N1-C2-O2	5.14	121.98	118.90
1	A	1314	C	C5-C4-N4	-5.14	116.60	120.20
1	A	1123	A	C2-N3-C4	5.13	113.17	110.60
1	A	1120	G	N9-C4-C5	-5.13	103.35	105.40
1	A	481	G	N3-C4-C5	-5.13	126.04	128.60
1	A	529	G	C6-C5-N7	-5.13	127.32	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1323	G	N9-C4-C5	-5.13	103.35	105.40
1	A	877	C	C6-N1-C2	5.12	122.35	120.30
1	A	1527	C	N1-C2-O2	5.12	121.97	118.90
1	A	995	C	N3-C2-O2	-5.12	118.32	121.90
1	A	1028	C	N3-C2-O2	-5.12	118.32	121.90
1	A	169	C	C4-C5-C6	5.11	119.96	117.40
1	A	1205	U	N3-C2-O2	-5.11	118.62	122.20
1	A	1006	C	C5-C6-N1	5.11	123.56	121.00
1	A	980	C	C5-C6-N1	5.11	123.55	121.00
1	A	968	A	N1-C6-N6	5.10	121.66	118.60
1	A	366	C	C5-C6-N1	-5.09	118.45	121.00
1	A	560	U	C5-C6-N1	5.09	125.25	122.70
1	A	1242	C	C2-N1-C1'	5.09	124.39	118.80
1	A	1215	G	C6-C5-N7	-5.08	127.35	130.40
1	A	1368	G	C5-C6-O6	-5.08	125.55	128.60
1	A	1030(A)	G	C8-N9-C4	-5.08	104.37	106.40
1	A	40	C	C2-N3-C4	-5.07	117.36	119.90
1	A	1003	G	C8-N9-C1'	5.07	133.60	127.00
1	A	889	A	C5-C6-N6	-5.07	119.65	123.70
1	A	500	G	N3-C4-C5	-5.06	126.07	128.60
1	A	1518	A	N9-C4-C5	5.06	107.82	105.80
1	A	517	G	C8-N9-C4	-5.05	104.38	106.40
1	A	1097	C	C6-N1-C2	-5.05	118.28	120.30
1	A	1005	A	C8-N9-C4	-5.05	103.78	105.80
1	A	1007	C	C5-C6-N1	5.05	123.53	121.00
1	A	355	C	N1-C2-O2	-5.05	115.87	118.90
1	A	1072	G	C8-N9-C4	-5.05	104.38	106.40
1	A	1151	A	N9-C4-C5	5.05	107.82	105.80
1	A	1153	C	C2-N3-C4	5.04	122.42	119.90
1	A	1037	C	C6-N1-C1'	5.04	126.85	120.80
1	A	1045	C	C5-C6-N1	5.04	123.52	121.00
1	A	307	C	N3-C4-C5	-5.04	119.89	121.90
1	A	483	C	C6-N1-C2	5.03	122.31	120.30
1	A	1093	A	N7-C8-N9	5.03	116.31	113.80
1	A	203	U	C5-C6-N1	5.02	125.21	122.70
1	A	531	U	N1-C2-O2	5.02	126.31	122.80
1	A	559	A	C8-N9-C4	-5.02	103.79	105.80
1	A	1004	A	C4-N9-C1'	5.02	135.33	126.30
1	A	1198	G	C6-C5-N7	5.01	133.41	130.40
1	A	770	C	N1-C2-O2	-5.01	115.89	118.90
1	A	1399	C	N3-C4-C5	-5.01	119.90	121.90
1	A	870	U	C6-N1-C2	5.01	124.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	128	GLU	Peptide
2	B	14	GLY	Peptide
2	B	71	VAL	Peptide
3	C	19	GLU	Peptide
3	C	46	GLU	Peptide
5	E	64	ARG	Peptide
7	G	57	GLU	Peptide
9	I	24	GLY	Peptide
12	L	91	LYS	Mainchain
13	M	66	LEU	Peptide
17	Q	33	GLY	Peptide
20	T	10	LEU	Peptide
22	V	26	LYS	Peptide
22	V	28	MET	Peptide
22	V	30	PRO	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	32270	0	16287	982	0
2	B	1775	0	1743	93	0
3	C	1450	0	1314	99	0
4	D	1526	0	1415	91	0
5	E	1105	0	1130	60	0
6	F	777	0	737	23	0
7	G	1164	0	1106	54	0
8	H	1045	0	1033	52	0
9	I	852	0	742	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	663	0	558	30	0
11	K	828	0	822	31	0
12	L	905	0	916	44	0
13	M	804	0	752	47	0
14	N	478	0	497	35	0
15	O	724	0	749	29	0
16	P	651	0	638	35	0
17	Q	823	0	891	18	0
18	R	514	0	530	24	0
19	S	560	0	466	23	0
20	T	713	0	766	30	0
21	U	199	0	208	9	0
22	V	353	0	266	13	0
23	A	71	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	120	0	0	13	0
25	D	1	0	0	0	0
25	K	2	0	0	0	0
25	P	1	0	0	0	0
25	T	2	0	0	0	0
All	All	50378	0	33566	1672	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 21.

All (1672) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:559:A:H4'	1:A:560:U:H3'	1.36	1.07
1:A:1003:G:H1	1:A:1037:C:N4	1.56	1.02
1:A:1010:G:H2'	1:A:1011:G:H8	1.28	0.98
1:A:1010:G:H2'	1:A:1011:G:C8	2.00	0.96
1:A:346:G:N2	1:A:347:G:N3	2.15	0.95
1:A:1164:G:H1	1:A:1172:C:H42	1.01	0.94
1:A:1003:G:N2	1:A:1037:C:N3	2.17	0.93
1:A:1164:G:H1	1:A:1172:C:N4	1.67	0.92
1:A:1237:C:H42	1:A:1337:G:H1	1.16	0.92
1:A:1047:G:H1	1:A:1210:C:H42	1.13	0.90
18:R:69:THR:HA	18:R:72:ARG:HD2	1.54	0.88
1:A:1047:G:H1	1:A:1210:C:N4	1.69	0.88
1:A:839:U:H5''	1:A:840:C:H5	1.39	0.87
1:A:1350:A:H61	1:A:1372:U:H3	1.21	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1273:G:H3'	1:A:1274:G:H8	1.38	0.87
22:V:4:GLN:NE2	22:V:4:GLN:O	2.06	0.87
1:A:677:U:H3	1:A:713:G:H22	1.22	0.86
5:E:122:GLU:O	5:E:126:ARG:NH1	2.08	0.85
19:S:50:ALA:HA	19:S:59:PRO:HA	1.58	0.85
7:G:74:GLU:OE1	7:G:95:ARG:NH2	2.08	0.85
1:A:1014:A:H2'	1:A:1015:A:C8	2.12	0.85
14:N:29:ARG:HD2	14:N:31:ARG:HB2	1.57	0.84
1:A:390:C:O3'	16:P:28:ARG:NH2	2.10	0.84
1:A:1380:U:O2	1:A:1382:C:N4	2.09	0.84
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.60	0.84
15:O:82:ILE:HB	15:O:87:ILE:HG22	1.61	0.83
1:A:557:G:OP1	25:A:1762:HOH:O	1.96	0.83
1:A:768:A:OP2	25:A:1757:HOH:O	1.96	0.82
3:C:137:ALA:HA	3:C:140:ARG:HD3	1.61	0.82
1:A:1346:A:H61	1:A:1374:A:H3'	1.43	0.82
1:A:136:C:H42	1:A:227:G:H1	1.25	0.82
1:A:1129:C:N4	1:A:1134:G:O6	2.13	0.81
3:C:141:VAL:HG11	3:C:202:ILE:HD12	1.62	0.81
5:E:76:ILE:HG13	5:E:77:PRO:HD2	1.63	0.81
1:A:1003:G:H1	1:A:1037:C:H42	0.82	0.81
1:A:1131:G:O6	1:A:1143:G:N2	2.13	0.81
1:A:511:C:H42	1:A:540:G:H1	1.27	0.80
1:A:559:A:OP1	5:E:126:ARG:NH2	2.13	0.80
1:A:854:G:N7	25:A:1776:HOH:O	2.13	0.80
1:A:405:U:O4	4:D:2:GLY:N	2.14	0.80
1:A:1502:A:H2	1:A:1505:G:H1	1.28	0.80
1:A:426:G:OP1	4:D:38:TYR:OH	1.99	0.80
5:E:43:LEU:O	5:E:65:ASN:ND2	2.14	0.79
1:A:1029:C:H1'	1:A:1032:G:H22	1.46	0.79
1:A:1075:C:OP1	2:B:179:LYS:NZ	2.16	0.79
1:A:1015:A:H1'	1:A:1219:U:H5'	1.65	0.79
6:F:11:ASN:HB3	6:F:14:LEU:HG	1.65	0.79
1:A:191:G:H21	20:T:103:GLY:HA2	1.45	0.79
4:D:13:ARG:NH1	4:D:38:TYR:O	2.16	0.78
1:A:537:G:N7	25:A:1769:HOH:O	2.15	0.78
1:A:17:U:H2'	1:A:18:C:C6	2.18	0.78
8:H:91:ARG:HD3	17:Q:33:GLY:HA3	1.66	0.78
1:A:1442(A):G:H2'	1:A:1442(B):A:H5'	1.65	0.77
12:L:76:ASN:ND2	12:L:106:ASP:O	2.17	0.77
16:P:53:VAL:HG13	16:P:79:VAL:HG22	1.64	0.77
3:C:35:GLU:HA	3:C:38:ARG:HD2	1.64	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1015:A:N3	1:A:1218:C:O2'	2.18	0.77
4:D:128:VAL:HG13	4:D:129:ASN:HD22	1.49	0.77
1:A:1441:G:H4'	1:A:1442:G:C8	2.19	0.77
7:G:89:MET:HG2	7:G:155:ARG:HG3	1.65	0.77
1:A:1160:G:H1	1:A:1176:A:H61	1.33	0.77
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.20	0.77
1:A:1047:G:N2	1:A:1210:C:N3	2.32	0.76
4:D:9:CYS:HA	4:D:12:CYS:HB2	1.66	0.76
1:A:1237:C:N4	1:A:1337:G:H1	1.84	0.76
2:B:139:LYS:HA	2:B:142:LEU:HB3	1.68	0.76
1:A:346:G:H21	1:A:347:G:H1'	1.50	0.76
16:P:28:ARG:HH11	16:P:28:ARG:HG2	1.49	0.76
1:A:1120:G:O6	1:A:1152:A:N6	2.19	0.76
2:B:136:VAL:HA	2:B:139:LYS:HG3	1.66	0.75
5:E:9:LYS:H	5:E:112:LEU:HD11	1.51	0.75
1:A:1118:C:H1'	1:A:1179:A:C4	2.21	0.75
1:A:1255:G:O6	10:J:43:ARG:NH2	2.20	0.75
21:U:15:ARG:HH11	21:U:15:ARG:HB2	1.50	0.75
1:A:426:G:OP1	4:D:36:ARG:NH1	2.20	0.75
1:A:1347:G:O2'	1:A:1373:G:O6	2.03	0.75
2:B:178:ARG:HH22	8:H:68:ARG:HH22	1.35	0.75
1:A:1122:U:H2'	1:A:1123:A:H8	1.52	0.75
1:A:673:G:H2'	1:A:674:G:C8	2.21	0.75
9:I:9:ARG:HG2	9:I:14:VAL:HG22	1.69	0.75
8:H:87:SER:HA	8:H:93:VAL:HG23	1.69	0.74
9:I:18:PHE:HB3	9:I:20:ARG:HE	1.50	0.74
13:M:108:ARG:HH21	13:M:114:ARG:HH11	1.35	0.74
1:A:10:A:H2'	1:A:11:G:H8	1.52	0.74
2:B:130:ARG:HA	2:B:130:ARG:HE	1.52	0.74
1:A:1028:C:N4	1:A:1034:G:N3	2.36	0.74
1:A:1387:G:H2'	1:A:1388:C:H6	1.52	0.74
1:A:1274:G:N2	1:A:1275:A:H62	1.86	0.74
10:J:49:VAL:HG21	14:N:45:ARG:HD2	1.70	0.73
1:A:999:C:H42	1:A:1042:G:H1	1.36	0.73
10:J:58:ASP:OD2	10:J:58:ASP:N	2.21	0.73
3:C:50:ALA:HB1	3:C:70:VAL:HG13	1.69	0.73
1:A:522:C:H5''	12:L:120:TYR:OH	1.88	0.73
1:A:1293:G:HO2'	1:A:1294:G:H8	1.33	0.73
1:A:1107:C:H5''	3:C:173:VAL:H	1.53	0.73
1:A:598:U:H4'	8:H:94:TYR:CD2	2.24	0.73
1:A:427:U:OP1	4:D:13:ARG:NH2	2.20	0.73
22:V:53:VAL:HG13	22:V:54:MET:HG3	1.70	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:542:G:OP1	4:D:10:ARG:NH1	2.23	0.72
1:A:991:U:C4	1:A:1212:U:H1'	2.25	0.72
2:B:155:LEU:HD11	2:B:159:PRO:HD3	1.71	0.72
1:A:1442:G:O2'	1:A:1442(A):G:OP1	2.07	0.72
1:A:1321:C:H5''	1:A:1322:C:H2'	1.71	0.72
13:M:104:ARG:HG3	13:M:105:THR:HG23	1.71	0.72
1:A:542:G:P	4:D:10:ARG:HH22	2.12	0.72
12:L:60:LEU:HD21	12:L:66:VAL:HG22	1.70	0.72
19:S:39:THR:OG1	19:S:70:LYS:NZ	2.22	0.72
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.53	0.72
1:A:1129:C:H4'	1:A:1130:A:H5'	1.71	0.72
1:A:1442:G:N7	1:A:1442(A):G:C6	2.58	0.72
1:A:973:G:H3'	1:A:974:A:H5''	1.72	0.72
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.71	0.71
1:A:1073:U:H2'	1:A:1074:G:C8	2.25	0.71
3:C:155:GLY:HA3	3:C:196:LEU:HD13	1.71	0.71
1:A:59:A:H5'	1:A:60:A:H5''	1.72	0.71
1:A:1286:A:C6	1:A:1354:C:H5''	2.25	0.71
4:D:79:PHE:HD2	4:D:80:GLU:H	1.35	0.71
13:M:47:ASP:N	13:M:47:ASP:OD1	2.22	0.71
1:A:1347:G:H8	9:I:107:ARG:HB3	1.55	0.71
5:E:98:THR:HB	5:E:117:ASP:HB3	1.72	0.71
8:H:45:ILE:HG22	8:H:63:LEU:HA	1.72	0.71
1:A:539:A:H2'	1:A:540:G:C8	2.26	0.71
3:C:114:PRO:O	3:C:118:GLN:NE2	2.25	0.70
1:A:1304:G:H1'	1:A:1333:A:H61	1.57	0.70
7:G:51:GLN:HG2	7:G:58:PRO:HD3	1.73	0.70
4:D:14:ARG:HA	4:D:39:PRO:HB3	1.74	0.70
1:A:1237:C:H3'	1:A:1336:C:H41	1.55	0.70
1:A:353:A:H5'	1:A:353:A:H8	1.56	0.70
1:A:1279:A:O2'	1:A:1281:U:OP2	2.08	0.69
1:A:1178:G:N2	1:A:1181:G:OP2	2.26	0.69
4:D:107:ARG:HE	4:D:173:TRP:HZ2	1.37	0.69
1:A:1142:G:H3'	1:A:1143:G:H8	1.58	0.69
1:A:1350:A:N6	1:A:1372:U:H3	1.91	0.69
1:A:1373:G:H5'	7:G:36:LYS:HB2	1.75	0.69
4:D:53:ASP:HB3	4:D:57:ARG:HH12	1.58	0.69
9:I:3:GLN:HB3	9:I:20:ARG:HG3	1.73	0.69
15:O:29:VAL:HG11	15:O:81:LEU:HD21	1.74	0.69
11:K:79:SER:HA	11:K:104:GLN:HB2	1.73	0.69
7:G:46:ALA:HB1	7:G:121:ALA:HB2	1.75	0.69
3:C:150:LYS:HB2	3:C:173:VAL:HG11	1.74	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:501:C:H2'	1:A:502:G:H8	1.58	0.69
9:I:96:LEU:HA	9:I:100:GLY:H	1.57	0.69
1:A:1004:A:N6	1:A:1035:A:N7	2.40	0.68
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.73	0.68
1:A:1264:C:H2'	1:A:1265:G:C8	2.28	0.68
10:J:54:PHE:CD2	10:J:55:LYS:HG3	2.28	0.68
1:A:1274:G:H21	1:A:1275:A:H62	1.39	0.68
1:A:584:G:H5'	17:Q:91:ARG:HH22	1.58	0.68
1:A:457:C:H2'	1:A:458:C:C6	2.29	0.68
2:B:185:ILE:HG22	2:B:199:TYR:HB2	1.75	0.68
1:A:448:A:OP2	1:A:485:G:N1	2.16	0.68
1:A:574:A:OP2	25:A:1793:HOH:O	2.11	0.68
5:E:43:LEU:HD21	5:E:132:ALA:HB1	1.76	0.68
1:A:377:G:OP1	16:P:3:LYS:NZ	2.24	0.68
3:C:177:THR:HB	3:C:180:ALA:HB2	1.75	0.68
1:A:1095:U:OP1	1:A:1108:G:N2	2.24	0.68
3:C:12:LEU:HD11	14:N:51:GLY:HA3	1.75	0.68
1:A:940:C:H42	1:A:1343:G:H1	1.42	0.68
4:D:127:THR:HG23	4:D:147:ALA:HB3	1.76	0.68
2:B:135:GLN:HA	2:B:138:LEU:HD12	1.76	0.68
1:A:49:U:H3	1:A:362:G:H1'	1.58	0.68
4:D:193:ASP:N	4:D:193:ASP:OD1	2.27	0.67
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.75	0.67
1:A:1285:A:H4'	1:A:1286:A:O5'	1.93	0.67
1:A:1084:G:H5''	1:A:1086:U:C4	2.27	0.67
1:A:148:G:H2'	1:A:149:A:H8	1.60	0.67
1:A:650:G:O6	25:A:1791:HOH:O	2.10	0.67
1:A:1287:A:H2'	1:A:1288:A:C8	2.30	0.67
9:I:71:SER:HA	9:I:74:ILE:HD12	1.74	0.67
14:N:29:ARG:HG3	14:N:31:ARG:H	1.60	0.67
1:A:1441:G:O2'	1:A:1459:C:N3	2.19	0.67
1:A:1073:U:H2'	1:A:1074:G:H8	1.60	0.67
4:D:80:GLU:O	4:D:83:SER:N	2.27	0.67
15:O:15:PHE:HE2	15:O:84:LYS:HD2	1.60	0.67
1:A:1502:A:H2	1:A:1505:G:N1	1.92	0.67
13:M:108:ARG:HE	13:M:114:ARG:HD3	1.60	0.67
1:A:1014:A:H8	1:A:1014:A:OP1	1.76	0.67
1:A:1309:G:OP2	13:M:99:ARG:NH2	2.24	0.67
6:F:91:VAL:HG11	18:R:72:ARG:HH12	1.60	0.66
1:A:1071:C:H2'	1:A:1072:G:H8	1.60	0.66
1:A:346:G:N2	1:A:347:G:H1'	2.09	0.66
9:I:9:ARG:HH11	9:I:9:ARG:HB2	1.59	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1530:G:OP1	25:A:1774:HOH:O	2.12	0.66
3:C:152:ILE:HG13	3:C:199:LYS:HD2	1.76	0.66
1:A:1028:C:N3	1:A:1034:G:H1'	2.10	0.66
1:A:1053:G:N7	1:A:1200:C:H5'	2.10	0.66
1:A:976:G:OP1	14:N:32:SER:N	2.18	0.66
1:A:436:C:H5''	4:D:156:GLU:OE2	1.96	0.66
6:F:100:ASN:ND2	18:R:23:LYS:O	2.28	0.66
1:A:674:G:H2'	1:A:675:A:H8	1.60	0.66
1:A:1147:C:O2	9:I:16:ARG:NH1	2.29	0.66
1:A:285:G:N7	25:A:1730:HOH:O	2.29	0.66
13:M:65:LYS:HA	13:M:66:LEU:HB2	1.76	0.66
1:A:538:G:H5''	12:L:114:LYS:HB2	1.77	0.66
4:D:173:TRP:CD1	4:D:174:LEU:HG	2.31	0.66
22:V:18:GLN:HE21	22:V:19:ALA:N	1.93	0.66
1:A:1106:G:H5'	3:C:172:ARG:HD2	1.77	0.65
10:J:53:PRO:O	14:N:41:ARG:NH2	2.30	0.65
20:T:16:HIS:O	20:T:19:SER:OG	2.13	0.65
7:G:20:ASP:HB3	7:G:23:VAL:HB	1.78	0.65
19:S:31:ILE:HG12	19:S:49:ILE:HG22	1.78	0.65
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.31	0.65
1:A:1264:C:N3	1:A:1271:G:O6	2.29	0.65
2:B:47:THR:HA	2:B:202:PRO:HG2	1.77	0.65
1:A:662:G:H2'	1:A:663:A:C8	2.31	0.65
15:O:62:GLN:HA	15:O:65:ARG:HD2	1.77	0.65
1:A:1244:C:H2'	1:A:1245:A:C8	2.31	0.65
1:A:434:U:H2'	1:A:435:C:C6	2.32	0.65
1:A:130:A:H5'	17:Q:63:ARG:HH21	1.60	0.65
1:A:537:G:H5''	12:L:113:ARG:NH1	2.12	0.65
1:A:881:G:P	12:L:12:ARG:HH22	2.19	0.65
1:A:620:C:H5''	25:A:1783:HOH:O	1.97	0.65
3:C:109:PRO:HA	3:C:112:SER:HB3	1.78	0.64
1:A:1442(A):G:C2'	1:A:1442(B):A:H5'	2.27	0.64
1:A:1027:C:C2	1:A:1034:G:N2	2.66	0.64
1:A:1222:G:OP2	1:A:1322:C:N4	2.24	0.64
4:D:14:ARG:HB2	4:D:40:PRO:HD2	1.79	0.64
1:A:1459:C:C6	1:A:1460:A:N7	2.66	0.64
3:C:31:HIS:HA	3:C:34:LEU:HB3	1.80	0.64
1:A:1280:A:H5'	10:J:41:PRO:HG2	1.78	0.64
1:A:524:G:H2'	1:A:525:C:C6	2.33	0.64
5:E:11:ILE:HG21	5:E:105:VAL:HG22	1.80	0.64
4:D:65:ARG:HG2	4:D:75:PHE:CD1	2.33	0.64
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.78	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:78:HIS:HE1	5:E:142:LEU:HA	1.62	0.64
1:A:1277:C:HO2'	1:A:1279:A:H8	1.46	0.64
1:A:1392:G:H21	1:A:1502:A:H8	1.43	0.64
9:I:17:VAL:HG13	9:I:63:ILE:HG12	1.78	0.64
18:R:31:LEU:HD12	18:R:66:LEU:HD13	1.79	0.64
18:R:70:ILE:O	18:R:74:ARG:HG3	1.97	0.64
1:A:841:U:H5	1:A:848:C:H1'	1.63	0.64
1:A:1308:U:H2'	1:A:1309:G:C8	2.33	0.63
1:A:600:C:H2'	1:A:601:C:C6	2.33	0.63
1:A:1375:A:H4'	7:G:29:LYS:HE2	1.80	0.63
1:A:1372:U:H2'	1:A:1373:G:O4'	1.97	0.63
13:M:96:LEU:HD23	13:M:97:PRO:HD2	1.80	0.63
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.63	0.63
2:B:208:ILE:HA	2:B:211:ILE:HD12	1.80	0.63
8:H:7:ALA:HB2	8:H:85:ARG:HG3	1.81	0.63
1:A:1302:U:OP2	13:M:21:TYR:OH	2.05	0.63
9:I:108:VAL:HG12	9:I:109:VAL:H	1.64	0.63
5:E:18:ARG:HH12	5:E:25:ARG:HD3	1.64	0.63
3:C:150:LYS:HG3	3:C:173:VAL:HG21	1.81	0.63
1:A:258:G:O6	25:A:1733:HOH:O	2.11	0.63
1:A:201:C:H42	1:A:216:G:H1	1.45	0.63
4:D:12:CYS:HA	4:D:19:LEU:HB2	1.80	0.63
1:A:859:A:H2'	1:A:860:A:O4'	1.99	0.63
8:H:33:GLU:HA	8:H:36:LEU:HD12	1.80	0.62
3:C:13:GLY:HA3	14:N:57:ARG:NH2	2.14	0.62
4:D:13:ARG:HB2	4:D:40:PRO:HD3	1.80	0.62
1:A:1308:U:H2'	1:A:1309:G:H8	1.63	0.62
1:A:1080:A:OP1	5:E:14:ARG:NH2	2.31	0.62
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.82	0.62
1:A:1027:C:H2'	1:A:1028:C:H5	1.65	0.62
1:A:346:G:N3	1:A:347:G:H1'	2.13	0.62
1:A:59:A:H3'	1:A:331:G:H22	1.64	0.62
1:A:1096:C:H2'	1:A:1097:C:H6	1.62	0.62
1:A:828:A:N6	1:A:858:G:O2'	2.32	0.62
1:A:38:G:C2	1:A:397:A:C2	2.87	0.62
2:B:127:ILE:HA	2:B:130:ARG:HG2	1.82	0.62
1:A:503:C:OP2	12:L:116:SER:HB3	1.99	0.62
1:A:524:G:H2'	1:A:525:C:H6	1.63	0.62
1:A:45:U:H3	1:A:396:G:H1	1.47	0.62
1:A:1235:U:H5''	21:U:3:LYS:HB2	1.81	0.62
1:A:1115:C:N3	1:A:1185:G:O6	2.33	0.62
2:B:80:ILE:HD13	2:B:212:GLN:HG2	1.81	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:15:PRO:HB2	16:P:41:PRO:HG3	1.82	0.62
1:A:1391:U:H2'	1:A:1392:G:C8	2.35	0.62
1:A:1359:C:H2'	1:A:1361:G:OP2	2.00	0.62
2:B:174:VAL:O	2:B:178:ARG:HB2	1.99	0.62
1:A:1070:U:O5'	5:E:25:ARG:NH1	2.32	0.62
1:A:590:C:H2'	1:A:591:U:H6	1.65	0.62
3:C:54:ARG:HD3	3:C:56:ASP:HB2	1.82	0.62
1:A:1513:A:H2'	1:A:1514:C:C6	2.35	0.62
1:A:1001:A:H2'	1:A:1001(A):G:C8	2.34	0.61
1:A:1459:C:N3	1:A:1460:A:N6	2.48	0.61
2:B:130:ARG:HB2	2:B:135:GLN:OE1	2.00	0.61
1:A:365:U:H5''	1:A:366:C:OP1	2.00	0.61
10:J:50:ILE:HA	10:J:60:ARG:HB3	1.82	0.61
1:A:833:U:H2'	1:A:834:C:H6	1.64	0.61
1:A:222:U:H2'	1:A:223:U:C6	2.36	0.61
1:A:629:G:H2'	1:A:630:G:O4'	2.00	0.61
2:B:195:ASP:O	8:H:74:PRO:HG3	2.01	0.61
2:B:213:LEU:HD22	2:B:214:ILE:HD13	1.80	0.61
15:O:15:PHE:CE2	15:O:84:LYS:HD2	2.35	0.61
5:E:33:VAL:HG21	5:E:109:ILE:HA	1.81	0.61
1:A:565:U:OP2	1:A:566:G:O2'	2.18	0.61
3:C:121:ALA:HB2	3:C:198:VAL:HG11	1.81	0.61
10:J:8:LEU:HB3	10:J:96:ILE:HG22	1.83	0.61
1:A:1348:U:O3'	9:I:120:ARG:HB2	2.00	0.61
9:I:27:THR:HA	9:I:32:ASP:HA	1.83	0.61
1:A:1347:G:C8	9:I:107:ARG:HB3	2.36	0.61
1:A:878:G:H5'	8:H:89:PRO:HG2	1.83	0.61
9:I:32:ASP:O	9:I:36:TYR:HB3	2.01	0.61
1:A:153:C:H2'	1:A:154:C:H6	1.64	0.61
1:A:1072:G:H2'	1:A:1073:U:C6	2.35	0.61
3:C:118:GLN:HA	3:C:121:ALA:HB3	1.81	0.61
1:A:625:G:H4'	16:P:16:HIS:CD2	2.35	0.61
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.83	0.61
1:A:1079:G:H2'	1:A:1080:A:C8	2.35	0.61
1:A:1118:C:H2'	1:A:1119:C:C6	2.35	0.61
1:A:445:G:H2'	1:A:446:G:C8	2.36	0.61
7:G:80:VAL:HG21	7:G:85:TYR:CD1	2.36	0.60
1:A:623:C:H2'	1:A:624:C:H6	1.66	0.60
1:A:1090:U:H2'	1:A:1091:U:H6	1.66	0.60
1:A:1278:U:H5''	1:A:1279:A:O4'	2.01	0.60
1:A:662:G:H2'	1:A:663:A:H8	1.66	0.60
1:A:450:G:OP1	16:P:43:LYS:NZ	2.33	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1162:C:H2'	1:A:1163:C:O4'	2.01	0.60
15:O:33:THR:HG21	15:O:85:LEU:HD22	1.82	0.60
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.82	0.60
7:G:26:PHE:HD1	7:G:101:LEU:HB3	1.67	0.60
13:M:88:ARG:CZ	13:M:88:ARG:HB2	2.31	0.60
1:A:1035:A:H2'	1:A:1036:G:H8	1.66	0.60
1:A:539:A:H2'	1:A:540:G:H8	1.65	0.60
1:A:475:G:H2'	1:A:476:G:H8	1.66	0.60
2:B:189:ASP:OD1	2:B:189:ASP:N	2.35	0.60
1:A:975:A:O2'	14:N:32:SER:HA	2.01	0.60
14:N:22:THR:HG22	14:N:35:ARG:HH21	1.67	0.60
20:T:72:LEU:HD21	20:T:77:ALA:HB2	1.83	0.60
1:A:1122:U:H2'	1:A:1123:A:C8	2.36	0.60
4:D:108:LEU:HD21	4:D:183:GLY:HA3	1.83	0.60
1:A:221:C:H2'	1:A:222:U:C6	2.36	0.60
1:A:1208:C:H2'	1:A:1209:C:H6	1.67	0.60
1:A:1133:G:H2'	1:A:1134:G:H8	1.66	0.60
1:A:1149:C:H2'	1:A:1150:U:O4'	2.01	0.60
3:C:114:PRO:HA	3:C:185:GLY:HA3	1.84	0.60
11:K:85:ARG:HD3	11:K:113:PRO:HD3	1.83	0.60
3:C:35:GLU:O	3:C:38:ARG:HB2	2.02	0.60
2:B:187:LEU:HD23	2:B:201:ILE:HB	1.83	0.60
20:T:97:ALA:HB3	20:T:99:LEU:H	1.66	0.60
1:A:1025:U:O2	1:A:1036:G:O6	2.20	0.59
8:H:36:LEU:HA	8:H:39:LEU:HD23	1.84	0.59
1:A:625:G:H2'	1:A:626:U:C6	2.37	0.59
1:A:927:G:H1	1:A:1390:U:H3	1.50	0.59
3:C:52:LEU:HA	3:C:70:VAL:HA	1.83	0.59
1:A:598:U:H2'	1:A:599:C:H6	1.68	0.59
9:I:40:LEU:HB2	9:I:43:ALA:HB2	1.82	0.59
1:A:1036:G:H3'	1:A:1037:C:H6	1.66	0.59
1:A:1164:G:N2	1:A:1172:C:N3	2.45	0.59
1:A:1333:A:H2'	1:A:1334:G:O4'	2.02	0.59
2:B:21:ARG:HB3	2:B:39:ILE:HG12	1.85	0.59
1:A:346:G:C2	1:A:347:G:H1'	2.36	0.59
2:B:121:LEU:HD21	2:B:138:LEU:HD13	1.83	0.59
1:A:688:G:H2'	1:A:689:C:H6	1.67	0.59
4:D:60:GLU:HG2	4:D:202:LEU:HB2	1.84	0.59
11:K:48:ILE:H	11:K:48:ILE:HD13	1.67	0.59
10:J:13:HIS:HB3	10:J:68:HIS:CE1	2.37	0.59
1:A:10:A:H2'	1:A:11:G:C8	2.36	0.59
1:A:1057:G:H4'	3:C:197:GLY:H	1.68	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:108:LEU:HD12	4:D:174:LEU:HD13	1.84	0.59
1:A:934:C:O2'	1:A:1344:C:OP2	2.12	0.59
1:A:1247:U:H1'	1:A:1291:G:N2	2.17	0.59
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.37	0.59
1:A:1193:G:N7	3:C:3:ASN:ND2	2.51	0.59
1:A:1374:A:O2'	7:G:28:ASN:HB3	2.02	0.59
1:A:148:G:H2'	1:A:149:A:C8	2.38	0.59
1:A:1090:U:H2'	1:A:1091:U:C6	2.37	0.59
1:A:243:A:H4'	1:A:244:U:O5'	2.01	0.59
6:F:22:GLU:O	6:F:26:ILE:HG13	2.03	0.59
16:P:22:THR:HA	16:P:33:ILE:HG13	1.84	0.59
7:G:108:ALA:HA	7:G:111:ARG:HD2	1.84	0.59
1:A:1137:C:H4'	1:A:1138:G:N2	2.18	0.59
1:A:542:G:H5'	4:D:41:GLY:HA3	1.85	0.59
1:A:1004:A:O2'	1:A:1037:C:O2	2.16	0.59
1:A:1179:A:H2'	1:A:1180:A:O4'	2.02	0.59
1:A:1206:G:O2'	3:C:192:THR:O	2.19	0.59
8:H:89:PRO:HA	8:H:92:ARG:HE	1.68	0.58
1:A:826:C:H4'	8:H:12:ARG:HG3	1.85	0.58
17:Q:24:GLU:OE2	17:Q:37:LYS:HD3	2.03	0.58
20:T:12:ALA:O	20:T:15:ARG:HB2	2.04	0.58
5:E:37:ARG:HG2	5:E:37:ARG:HH11	1.68	0.58
1:A:1001(A):G:H2'	1:A:1002:G:H8	1.68	0.58
1:A:1346:A:H4'	1:A:1347:G:H4'	1.85	0.58
1:A:511:C:N4	1:A:540:G:H1	1.99	0.58
1:A:1317:C:N3	19:S:37:ARG:NH2	2.44	0.58
1:A:1012:U:H2'	1:A:1013:G:O4'	2.04	0.58
11:K:59:TYR:O	11:K:62:GLN:HB3	2.03	0.58
13:M:85:GLY:HA3	19:S:74:PHE:HA	1.83	0.58
7:G:85:TYR:HD1	7:G:154:TYR:HE1	1.51	0.58
1:A:512:U:H2'	1:A:513:C:C6	2.38	0.58
1:A:804:U:H5''	1:A:805:C:OP2	2.02	0.58
20:T:41:ILE:HA	20:T:44:ALA:HB3	1.86	0.58
1:A:1029:C:C2	1:A:1032:G:N1	2.72	0.58
1:A:841:U:C5	1:A:848:C:H1'	2.38	0.58
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.37	0.58
1:A:1411:C:H2'	1:A:1412:C:H6	1.69	0.58
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.84	0.58
10:J:55:LYS:O	10:J:57:LYS:N	2.35	0.58
1:A:149:A:O2'	1:A:150:C:H6	1.87	0.58
1:A:1290:G:H3'	1:A:1291:G:H8	1.69	0.58
1:A:428:G:H5''	4:D:7:PRO:HB3	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:501:C:H2'	1:A:502:G:C8	2.38	0.58
1:A:436:C:H4'	4:D:156:GLU:HB2	1.85	0.58
1:A:438:G:OP1	4:D:125:HIS:HE1	1.86	0.58
1:A:659:U:H2'	1:A:660:G:C8	2.39	0.58
1:A:1348:U:H4'	9:I:120:ARG:HD2	1.85	0.58
2:B:219:VAL:HA	2:B:222:ILE:HD12	1.86	0.58
12:L:32:PHE:HE1	12:L:86:ARG:HG3	1.67	0.58
1:A:203:U:H5''	1:A:204:U:OP2	2.04	0.58
1:A:1198:G:H2'	1:A:1199:U:C6	2.39	0.57
6:F:69:GLU:O	6:F:72:VAL:HG12	2.03	0.57
1:A:487:A:H2'	1:A:488:C:O4'	2.04	0.57
2:B:21:ARG:H	2:B:21:ARG:HD3	1.70	0.57
1:A:939:G:H1	1:A:1344:C:H42	1.52	0.57
20:T:13:LEU:O	20:T:17:ARG:HG3	2.04	0.57
3:C:51:GLY:HA3	3:C:71:ALA:HB3	1.87	0.57
4:D:119:GLN:HG2	4:D:123:HIS:CD2	2.39	0.57
1:A:991:U:O2'	1:A:992:U:O5'	2.15	0.57
1:A:552:U:H4'	12:L:86:ARG:HG2	1.84	0.57
1:A:325:A:OP2	20:T:70:SER:OG	2.19	0.57
1:A:984:C:H2'	1:A:985:C:H6	1.68	0.57
9:I:4:TYR:HD1	9:I:87:GLN:HG3	1.70	0.57
1:A:519:C:H2'	1:A:520:A:C8	2.39	0.57
3:C:54:ARG:HB3	3:C:69:HIS:HB2	1.86	0.57
1:A:708:C:OP1	11:K:85:ARG:NH2	2.37	0.57
1:A:327:A:HO2'	1:A:329:A:H8	1.53	0.57
1:A:736:C:H2'	1:A:737:A:C8	2.39	0.57
1:A:1163:C:C2	1:A:1164:G:C8	2.92	0.57
1:A:501:C:H1'	1:A:549:C:H1'	1.86	0.57
1:A:980:C:H1'	14:N:19:ARG:HA	1.87	0.57
1:A:15:G:H4'	5:E:24:ARG:HH12	1.70	0.57
1:A:269:C:H2'	1:A:270:A:C8	2.40	0.57
13:M:108:ARG:NE	13:M:114:ARG:HD3	2.19	0.57
3:C:125:GLU:HG3	3:C:189:ALA:HB1	1.86	0.57
1:A:164:U:H2'	1:A:165:C:C6	2.40	0.57
1:A:136:C:N4	1:A:227:G:H1	2.00	0.57
4:D:55:ALA:O	4:D:59:ARG:HG2	2.04	0.57
1:A:741:G:H2'	1:A:742:G:O4'	2.04	0.57
5:E:78:HIS:CE1	5:E:142:LEU:HD23	2.40	0.57
1:A:1076:C:H42	1:A:1081:G:H1	1.51	0.57
1:A:814:A:N7	1:A:816:A:C4	2.73	0.57
1:A:382:A:H2'	1:A:383:A:H8	1.69	0.57
1:A:1272:G:H2'	1:A:1273:G:H8	1.70	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1293:G:O2'	1:A:1294:G:H8	1.88	0.57
1:A:1281:U:H5''	1:A:1282:C:OP2	2.05	0.57
3:C:54:ARG:NH1	3:C:56:ASP:OD1	2.37	0.57
1:A:564:C:O2'	8:H:91:ARG:NH2	2.25	0.57
1:A:1072:G:H2'	1:A:1073:U:H6	1.69	0.57
1:A:1083:U:C5	1:A:1084:G:C6	2.92	0.57
4:D:108:LEU:HB3	4:D:110:PHE:CE1	2.40	0.57
13:M:92:HIS:NE2	13:M:98:VAL:HG21	2.20	0.57
1:A:868:C:H2'	1:A:869:G:O4'	2.05	0.57
20:T:33:ILE:O	20:T:37:SER:OG	2.20	0.57
13:M:4:ILE:O	13:M:6:GLY:N	2.38	0.57
1:A:7:G:O2'	5:E:120:THR:O	2.22	0.57
14:N:2:ALA:HB1	14:N:6:LEU:HD13	1.86	0.57
5:E:93:PRO:HG2	8:H:105:ARG:NE	2.20	0.56
2:B:103:THR:HG23	2:B:176:GLU:HB3	1.86	0.56
1:A:920:U:H2'	1:A:921:U:C6	2.41	0.56
16:P:20:VAL:HG23	16:P:35:LYS:HA	1.87	0.56
1:A:1255:G:O3'	1:A:1258:G:H1'	2.05	0.56
1:A:1330:U:H5'	1:A:1331:G:O5'	2.06	0.56
18:R:53:ARG:HE	18:R:59:SER:C	2.08	0.56
1:A:370:C:H2'	1:A:371:G:C8	2.40	0.56
1:A:1442(A):G:C8	1:A:1442(B):A:C2	2.93	0.56
8:H:112:LEU:HA	8:H:134:ILE:HG12	1.88	0.56
1:A:522:C:N4	1:A:528:C:H42	2.04	0.56
1:A:612:C:O2	1:A:629:G:N2	2.38	0.56
16:P:20:VAL:HG21	16:P:32:TYR:CG	2.40	0.56
2:B:98:LEU:HB2	2:B:101:MET:HE3	1.87	0.56
1:A:1218:C:H2'	1:A:1219:U:C6	2.39	0.56
1:A:1181:G:H4'	1:A:1184:G:O4'	2.05	0.56
2:B:185:ILE:HA	2:B:199:TYR:O	2.05	0.56
1:A:857:C:H2'	1:A:858:G:O4'	2.05	0.56
1:A:1003:G:H2'	1:A:1004:A:H4'	1.88	0.56
4:D:129:ASN:HD21	4:D:145:GLU:N	2.04	0.56
1:A:954:G:O6	13:M:104:ARG:NH1	2.39	0.56
3:C:19:GLU:O	3:C:40:ARG:NH2	2.38	0.56
1:A:346:G:H21	1:A:347:G:C1'	2.18	0.56
7:G:43:PHE:HD2	7:G:44:TYR:CE2	2.24	0.56
11:K:58:PRO:HA	11:K:90:GLY:HA2	1.88	0.56
1:A:1343:G:H4'	9:I:122:ALA:HB3	1.88	0.56
1:A:1356:G:H2'	1:A:1357:A:C8	2.41	0.56
1:A:1130:A:H61	1:A:1144:G:H1'	1.71	0.56
1:A:598:U:H2'	1:A:599:C:C6	2.41	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:939:G:H5''	7:G:102:ARG:CZ	2.35	0.56
1:A:153:C:H2'	1:A:154:C:C6	2.40	0.56
1:A:1095:U:H2'	1:A:1096:C:C6	2.41	0.56
1:A:458:C:H2'	1:A:460:G:H8	1.69	0.56
1:A:659:U:H2'	1:A:660:G:H8	1.69	0.56
1:A:639:G:H2'	1:A:640:A:H8	1.71	0.56
1:A:913:A:H4'	1:A:914:A:O5'	2.05	0.56
1:A:1287:A:H2'	1:A:1288:A:H8	1.71	0.56
1:A:221:C:H2'	1:A:222:U:H6	1.69	0.56
9:I:117:HIS:CE1	9:I:123:PRO:HG3	2.41	0.56
5:E:30:ALA:N	5:E:46:GLY:O	2.29	0.56
1:A:950:U:H1'	1:A:971:G:C5	2.41	0.55
1:A:160:A:H61	1:A:346:G:N2	2.05	0.55
2:B:18:GLY:HA3	2:B:41:ILE:HG23	1.87	0.55
1:A:1009:G:H1	1:A:1020:U:H1'	1.72	0.55
13:M:69:GLU:O	13:M:70:LEU:HB3	2.07	0.55
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.87	0.55
16:P:59:TRP:HA	16:P:62:VAL:HG12	1.87	0.55
3:C:43:LEU:O	3:C:47:LEU:N	2.39	0.55
3:C:113:ALA:HB2	3:C:202:ILE:HG12	1.88	0.55
3:C:88:ARG:O	3:C:92:ALA:HB3	2.06	0.55
13:M:14:ARG:HD2	13:M:42:ALA:O	2.05	0.55
1:A:346:G:N2	1:A:347:G:C4	2.75	0.55
1:A:35:G:C2	1:A:550:G:C2	2.94	0.55
1:A:1227:A:H8	1:A:1227:A:H5'	1.71	0.55
1:A:1459:C:H41	1:A:1461:G:N2	2.05	0.55
8:H:6:ILE:HB	8:H:85:ARG:HH12	1.70	0.55
8:H:4:ASP:HB2	8:H:89:PRO:HG3	1.88	0.55
1:A:993:G:N3	1:A:993:G:H2'	2.21	0.55
1:A:1300:G:O2'	1:A:1303:C:N4	2.40	0.55
10:J:11:PHE:CE2	10:J:67:THR:HB	2.42	0.55
1:A:79:G:H1	1:A:90:U:H3	1.55	0.55
7:G:47:CYS:O	7:G:58:PRO:HG3	2.05	0.55
1:A:819:A:H4'	1:A:820:U:OP2	2.07	0.55
1:A:1493:A:H4'	1:A:1494:G:OP1	2.06	0.55
3:C:5:ILE:HD12	3:C:6:HIS:H	1.72	0.55
11:K:33:THR:HA	11:K:39:PRO:HA	1.89	0.55
3:C:22:TRP:HA	10:J:93:GLY:HA2	1.88	0.55
8:H:81:HIS:ND1	8:H:138:TRP:OXT	2.34	0.55
1:A:592:G:H1	1:A:647:C:H42	1.55	0.55
1:A:979:C:H42	14:N:18:VAL:HG12	1.72	0.54
1:A:186:C:H2'	1:A:187:C:C6	2.42	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:59:TYR:CE1	13:M:63:THR:HG21	2.42	0.54
1:A:1095:U:P	1:A:1108:G:H1	2.30	0.54
1:A:955:U:H2'	1:A:956:U:O4'	2.07	0.54
1:A:969:A:OP1	10:J:55:LYS:NZ	2.31	0.54
21:U:3:LYS:HB3	21:U:14:TRP:CE3	2.42	0.54
3:C:20:SER:HB3	3:C:40:ARG:HH22	1.73	0.54
3:C:5:ILE:HD11	14:N:49:HIS:CE1	2.43	0.54
1:A:1063:C:H3'	1:A:1064:G:H2'	1.89	0.54
18:R:56:THR:HB	18:R:58:LEU:HD13	1.87	0.54
4:D:177:ASP:OD1	4:D:180:GLY:HA3	2.06	0.54
22:V:23:GLY:N	22:V:24:ARG:HA	2.22	0.54
4:D:59:ARG:HA	4:D:62:GLN:HB2	1.88	0.54
4:D:12:CYS:HA	4:D:19:LEU:HD23	1.89	0.54
17:Q:86:GLU:O	17:Q:90:ILE:HG12	2.07	0.54
8:H:120:THR:OG1	8:H:123:GLU:HG3	2.08	0.54
4:D:79:PHE:HD2	4:D:80:GLU:N	2.04	0.54
1:A:448:A:H2'	1:A:449:C:C6	2.42	0.54
1:A:1239:A:H2'	1:A:1298:C:H42	1.72	0.54
1:A:652:U:O4	1:A:752:G:O2'	2.20	0.54
1:A:262:A:H2'	1:A:263:A:C8	2.42	0.54
1:A:473:G:H2'	1:A:474:G:C8	2.43	0.54
5:E:57:LYS:O	5:E:61:TYR:HD2	1.90	0.54
22:V:27:GLU:H	22:V:44:TRP:HE1	1.54	0.54
5:E:126:ARG:HA	5:E:131:ILE:HD11	1.89	0.54
3:C:52:LEU:HD13	3:C:68:VAL:HG13	1.89	0.54
1:A:1292:U:H2'	1:A:1293:G:C8	2.42	0.54
1:A:1147:C:H2'	1:A:1148:U:C6	2.43	0.54
1:A:1046:A:H3'	1:A:1047:G:C8	2.43	0.54
1:A:833:U:H2'	1:A:834:C:C6	2.43	0.54
20:T:66:ALA:HB3	20:T:72:LEU:HD22	1.90	0.54
19:S:69:HIS:HD2	19:S:74:PHE:CE1	2.26	0.54
6:F:91:VAL:HG13	18:R:72:ARG:HH22	1.72	0.54
1:A:102:G:H2'	1:A:103:C:C6	2.43	0.54
1:A:396:G:O2'	1:A:398:C:OP1	2.17	0.54
20:T:43:LEU:O	20:T:47:GLY:N	2.33	0.54
1:A:673:G:O3'	6:F:87:ARG:NH2	2.41	0.54
1:A:839:U:H5''	1:A:840:C:C5	2.31	0.53
1:A:544:G:C6	1:A:545:C:C4	2.96	0.53
21:U:15:ARG:HG2	21:U:17:THR:HG23	1.89	0.53
8:H:85:ARG:NE	8:H:87:SER:O	2.41	0.53
2:B:24:TRP:CE3	2:B:26:PRO:HA	2.43	0.53
1:A:35:G:O2'	12:L:118:SER:O	2.25	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:404:U:H5'	4:D:122:ARG:HD3	1.89	0.53
13:M:13:LYS:O	13:M:45:VAL:HG23	2.08	0.53
1:A:1151:A:N3	10:J:39:PRO:HG2	2.22	0.53
1:A:1003:G:N2	1:A:1038:C:C4	2.77	0.53
2:B:211:ILE:HG22	2:B:215:LEU:HG	1.89	0.53
7:G:51:GLN:O	7:G:55:GLY:HA2	2.08	0.53
1:A:1277:C:O2'	1:A:1279:A:H8	1.91	0.53
1:A:1493:A:O2'	1:A:1494:G:O5'	2.24	0.53
1:A:304:U:H2'	1:A:305:G:C8	2.44	0.53
1:A:777:A:H2	11:K:119:CYS:HB3	1.72	0.53
12:L:102:ARG:HB3	12:L:108:ALA:O	2.08	0.53
8:H:85:ARG:HG3	8:H:85:ARG:HH11	1.74	0.53
1:A:999:C:N4	1:A:1042:G:H1	2.04	0.53
1:A:430:A:P	4:D:22:LYS:HZ3	2.30	0.53
1:A:100:C:H2'	1:A:101:A:C8	2.44	0.53
3:C:64:VAL:O	3:C:99:VAL:HA	2.09	0.53
6:F:27:GLN:HA	6:F:30:LEU:HD12	1.89	0.53
1:A:331:G:O4'	25:A:1724:HOH:O	2.19	0.53
1:A:828:A:H2'	1:A:829:G:O4'	2.08	0.53
21:U:15:ARG:NH1	21:U:15:ARG:HB2	2.21	0.53
7:G:43:PHE:O	7:G:47:CYS:N	2.42	0.53
1:A:1192:C:OP2	3:C:4:LYS:NZ	2.38	0.53
1:A:176:C:H2'	1:A:177:C:C6	2.44	0.53
1:A:181:G:O2'	1:A:183:G:N7	2.41	0.53
1:A:560:U:H4'	1:A:561:U:O5'	2.08	0.53
1:A:1130:A:N6	1:A:1144:G:N3	2.56	0.53
1:A:625:G:H2'	1:A:626:U:H6	1.73	0.53
1:A:1298:C:P	7:G:114:ARG:HH22	2.31	0.53
1:A:103:C:H1'	1:A:171:A:N1	2.23	0.53
12:L:34:ARG:O	12:L:61:THR:HG23	2.09	0.53
1:A:1504:G:H3'	1:A:1504:G:P	2.49	0.53
1:A:1132:C:H2'	1:A:1133:G:O4'	2.09	0.53
1:A:954:G:H21	1:A:1227:A:H62	1.57	0.53
1:A:583:A:H2'	1:A:584:G:O4'	2.09	0.53
1:A:1357:A:H3'	1:A:1358:U:C6	2.43	0.53
1:A:1142:G:H3'	1:A:1143:G:C8	2.41	0.53
1:A:964:A:N3	1:A:969:A:O2'	2.31	0.53
1:A:1192:C:N3	1:A:1193:G:H1'	2.24	0.53
1:A:1014:A:H5'	19:S:14:HIS:ND1	2.24	0.53
3:C:33:LEU:HG	3:C:34:LEU:N	2.23	0.53
3:C:12:LEU:HD11	14:N:51:GLY:CA	2.39	0.53
1:A:437:U:O3'	4:D:125:HIS:NE2	2.36	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1009:G:N2	1:A:1020:U:O2'	2.41	0.53
1:A:1131:G:H2'	1:A:1132:C:C6	2.44	0.53
9:I:4:TYR:CD1	9:I:87:GLN:HG3	2.44	0.53
3:C:122:GLU:HA	3:C:125:GLU:OE2	2.08	0.53
1:A:1353:G:H2'	1:A:1354:C:C6	2.44	0.52
21:U:9:ARG:O	21:U:13:ILE:HG13	2.09	0.52
1:A:1142:G:H2'	1:A:1143:G:O4'	2.08	0.52
1:A:1107:C:C4	1:A:1108:G:C8	2.97	0.52
1:A:428:G:H4'	1:A:429:U:O5'	2.09	0.52
9:I:95:LYS:O	9:I:99:LEU:N	2.34	0.52
13:M:31:LYS:HA	13:M:34:LEU:HB2	1.90	0.52
1:A:1192:C:N4	1:A:1193:G:N3	2.56	0.52
7:G:116:ALA:HA	7:G:119:ARG:HG3	1.90	0.52
2:B:201:ILE:HG21	2:B:214:ILE:HG21	1.90	0.52
1:A:818:G:O2'	1:A:819:A:H5'	2.10	0.52
18:R:37:VAL:HG12	18:R:78:LEU:HB3	1.91	0.52
1:A:1133:G:H2'	1:A:1134:G:C8	2.44	0.52
9:I:11:LYS:O	9:I:12:GLU:HB2	2.09	0.52
9:I:46:ALA:O	9:I:49:PRO:HD2	2.09	0.52
5:E:68:GLU:HG2	5:E:70:PRO:HD3	1.92	0.52
1:A:322:C:H4'	20:T:23:ARG:HD2	1.90	0.52
7:G:77:SER:HA	7:G:86:GLN:HA	1.91	0.52
8:H:124:ALA:HB1	8:H:129:VAL:O	2.10	0.52
13:M:91:ARG:HB2	13:M:98:VAL:HG13	1.90	0.52
2:B:18:GLY:HA2	2:B:42:ILE:HG13	1.90	0.52
1:A:737:A:H2'	1:A:738:C:C6	2.45	0.52
1:A:1362:C:H2'	1:A:1363:C:H5''	1.91	0.52
1:A:110:C:H2'	1:A:111:G:O4'	2.10	0.52
1:A:940:C:N4	1:A:1343:G:H1	2.07	0.52
1:A:1279:A:H61	3:C:26:LYS:HZ2	1.58	0.52
1:A:20:U:H2'	1:A:21:G:O4'	2.10	0.52
1:A:1004:A:H2'	1:A:1036:G:C6	2.44	0.52
1:A:160:A:H2'	1:A:161:A:O4'	2.10	0.52
1:A:1128:C:H5	1:A:1139:G:HO2'	1.54	0.52
9:I:17:VAL:HG22	9:I:63:ILE:HG23	1.91	0.52
4:D:134:ASP:OD2	4:D:135:LEU:HD13	2.10	0.52
1:A:538:G:OP2	12:L:115:LYS:HB2	2.10	0.52
1:A:673:G:H2'	1:A:674:G:H8	1.70	0.52
1:A:1277:C:H2'	1:A:1278:U:H5'	1.91	0.52
1:A:735:C:H2'	1:A:736:C:H6	1.75	0.52
1:A:1238:A:OP2	1:A:1300:G:N2	2.42	0.52
1:A:193:C:H2'	1:A:194:C:C6	2.45	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:18:TRP:CD1	14:N:54:PRO:HA	2.45	0.52
1:A:1084:G:H5''	1:A:1086:U:C5	2.44	0.52
1:A:626:U:C2	1:A:627:G:C8	2.97	0.52
1:A:473:G:H2'	1:A:474:G:H8	1.74	0.52
5:E:57:LYS:HB3	5:E:61:TYR:HE2	1.74	0.52
1:A:191:G:N2	20:T:103:GLY:HA2	2.20	0.51
1:A:1291:G:H4'	9:I:38:GLN:O	2.09	0.51
18:R:66:LEU:O	18:R:70:ILE:HG13	2.09	0.51
1:A:1234:C:H1'	1:A:1364:U:O2	2.10	0.51
9:I:4:TYR:CE2	9:I:88:TYR:HD1	2.27	0.51
4:D:110:PHE:CD1	4:D:110:PHE:N	2.77	0.51
1:A:626:U:H2'	1:A:627:G:H8	1.74	0.51
1:A:925:G:H5''	1:A:926:G:OP1	2.09	0.51
1:A:359:U:H2'	1:A:360:A:H8	1.74	0.51
1:A:1182:G:H4'	1:A:1183:A:C5'	2.41	0.51
4:D:110:PHE:HD1	4:D:110:PHE:N	2.09	0.51
3:C:13:GLY:HA3	14:N:57:ARG:HH22	1.75	0.51
20:T:54:LYS:HA	20:T:57:ARG:CZ	2.40	0.51
1:A:391:G:O3'	16:P:8:ARG:NH2	2.44	0.51
1:A:1133:G:H1	1:A:1141:C:H42	1.57	0.51
1:A:406:G:N3	4:D:119:GLN:NE2	2.57	0.51
9:I:18:PHE:HB3	9:I:20:ARG:NE	2.21	0.51
1:A:1071:C:H2'	1:A:1072:G:C8	2.44	0.51
1:A:1057:G:O3'	3:C:197:GLY:HA3	2.11	0.51
1:A:971:G:P	1:A:1231:G:H21	2.34	0.51
1:A:1092:A:C6	1:A:1183:A:H2	2.28	0.51
1:A:37:U:O2'	1:A:500:G:H4'	2.11	0.51
14:N:7:ILE:HA	14:N:23:ARG:HE	1.74	0.51
9:I:112:LYS:HA	9:I:119:ALA:CB	2.37	0.51
1:A:1107:C:C5'	3:C:173:VAL:H	2.23	0.51
16:P:15:PRO:HB3	16:P:17:TYR:HE1	1.76	0.51
1:A:1190:G:OP1	3:C:5:ILE:HG22	2.11	0.51
13:M:59:TYR:O	13:M:63:THR:HB	2.11	0.51
1:A:1063:C:H5''	1:A:1064:G:H3'	1.93	0.51
1:A:499:A:H4'	1:A:500:G:H5'	1.92	0.51
6:F:40:VAL:HG22	6:F:42:GLU:H	1.75	0.51
1:A:542:G:H2'	1:A:543:C:H6	1.75	0.51
13:M:65:LYS:HA	13:M:66:LEU:CB	2.41	0.51
1:A:382:A:H2'	1:A:383:A:C8	2.45	0.51
9:I:11:LYS:H	9:I:104:ARG:NH2	2.09	0.51
1:A:588:G:P	25:A:1787:HOH:O	2.69	0.51
1:A:1272:G:H2'	1:A:1273:G:C8	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:688:G:H2'	1:A:689:C:C6	2.46	0.51
3:C:68:VAL:HG12	3:C:70:VAL:HG23	1.92	0.51
4:D:3:ARG:O	4:D:5:ILE:HG12	2.10	0.51
1:A:303:A:HO2'	1:A:555:C:HO2'	1.57	0.51
1:A:950:U:H1'	1:A:971:G:C4	2.46	0.51
1:A:669:U:H2'	1:A:670:G:H8	1.76	0.51
3:C:18:TRP:HE1	14:N:55:GLY:N	2.09	0.51
1:A:266:G:H5''	1:A:267:C:C5	2.46	0.51
1:A:279:A:H4'	1:A:280:C:H5''	1.92	0.51
1:A:1486:G:H2'	1:A:1487:G:O4'	2.11	0.51
1:A:1003:G:H2'	1:A:1004:A:C4'	2.41	0.51
1:A:1441:G:H4'	1:A:1442:G:N7	2.25	0.51
1:A:327:A:O2'	1:A:329:A:H8	1.94	0.51
1:A:233:C:H2'	1:A:234:C:H6	1.75	0.51
2:B:16:HIS:HA	2:B:210:SER:OG	2.11	0.51
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.92	0.51
1:A:1028:C:N4	1:A:1034:G:C2	2.78	0.50
1:A:1237:C:N3	1:A:1337:G:N2	2.54	0.50
1:A:1160:G:H1	1:A:1176:A:N6	2.03	0.50
9:I:87:GLN:HA	9:I:87:GLN:HE21	1.76	0.50
1:A:21:G:H2'	1:A:22:G:C8	2.46	0.50
7:G:9:VAL:HG13	7:G:94:ARG:HH21	1.76	0.50
1:A:50:A:H1'	1:A:52:G:C8	2.45	0.50
1:A:69:G:C2	1:A:70:G:C5	2.99	0.50
1:A:1266:G:N2	1:A:1268:A:H8	2.08	0.50
1:A:1041:A:H2'	1:A:1042:G:O4'	2.10	0.50
1:A:664:G:P	18:R:64:ARG:HH21	2.33	0.50
1:A:196:A:N3	1:A:222:U:H1'	2.26	0.50
1:A:660:G:H2'	1:A:661:G:H8	1.76	0.50
11:K:30:VAL:HG21	11:K:65:ALA:HA	1.91	0.50
9:I:73:GLN:O	9:I:77:ILE:HG13	2.10	0.50
22:V:30:PRO:HB3	22:V:40:TRP:CD2	2.45	0.50
1:A:1400:C:H4'	1:A:1401:G:OP2	2.11	0.50
13:M:97:PRO:HD3	13:M:110:ARG:HB3	1.93	0.50
9:I:48:GLU:HB3	9:I:101:PHE:CZ	2.46	0.50
1:A:323:U:O3'	20:T:22:ARG:HD3	2.11	0.50
15:O:63:ARG:NH1	15:O:87:ILE:HD11	2.27	0.50
1:A:509:A:H3'	1:A:509:A:C8	2.46	0.50
1:A:1442(B):A:O2'	1:A:1443:G:OP2	2.24	0.50
1:A:169:C:C5	1:A:170:U:C4	2.99	0.50
2:B:149:LEU:HB3	2:B:152:PHE:HB3	1.92	0.50
1:A:636:U:H5'	17:Q:2:PRO:HG3	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:13:HIS:HB2	22:V:39:GLN:HG3	1.94	0.50
4:D:7:PRO:O	4:D:10:ARG:HB3	2.11	0.50
1:A:649:G:H2'	1:A:650:G:H8	1.76	0.50
1:A:841:U:OP2	1:A:841:U:C2	2.64	0.50
1:A:1458:G:N3	1:A:1458:G:H2'	2.27	0.50
1:A:1007:C:H2'	1:A:1008:C:H6	1.76	0.50
1:A:1015:A:H2	1:A:1218:C:O2	1.94	0.50
16:P:28:ARG:NH1	16:P:29:ASP:OD2	2.44	0.50
1:A:474:G:H2'	1:A:475:G:C8	2.47	0.50
1:A:203:U:H4'	1:A:204:U:OP1	2.11	0.50
9:I:18:PHE:HB2	9:I:62:TYR:HB3	1.94	0.50
1:A:450:G:H4'	16:P:41:PRO:HB2	1.93	0.50
1:A:1310:G:H1	1:A:1327:C:H42	1.60	0.50
18:R:36:ASN:HB2	18:R:39:VAL:HG23	1.94	0.50
4:D:64:LEU:HB2	4:D:198:VAL:HG11	1.92	0.50
1:A:982:U:N3	1:A:1223:C:N3	2.58	0.50
1:A:1387:G:H2'	1:A:1388:C:C6	2.39	0.50
1:A:192:U:H2'	1:A:193:C:C6	2.47	0.50
5:E:51:VAL:O	5:E:55:VAL:HG23	2.11	0.50
5:E:135:THR:O	5:E:138:ALA:HB3	2.11	0.50
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.93	0.50
1:A:1289:A:N1	1:A:1372:U:H5'	2.27	0.50
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.27	0.50
1:A:658:G:C6	1:A:659:U:C4	3.00	0.50
1:A:1068:G:N7	1:A:1094:G:C8	2.80	0.50
1:A:729:A:H2'	1:A:730:G:H8	1.75	0.50
1:A:1228:C:H2'	1:A:1229:A:H8	1.77	0.50
1:A:1338:G:H2'	1:A:1339:A:C8	2.47	0.49
7:G:88:PRO:HB3	7:G:145:ALA:HA	1.94	0.49
1:A:1014:A:H5'	19:S:14:HIS:CG	2.46	0.49
4:D:32:ALA:O	4:D:36:ARG:N	2.45	0.49
8:H:121:ASP:OD1	8:H:121:ASP:N	2.44	0.49
1:A:1003:G:C4	1:A:1004:A:H1'	2.46	0.49
10:J:55:LYS:C	10:J:57:LYS:H	2.15	0.49
1:A:1128:C:C5'	9:I:16:ARG:HH12	2.24	0.49
1:A:1208:C:H2'	1:A:1209:C:C6	2.47	0.49
1:A:109:A:C6	1:A:326:G:C6	3.00	0.49
6:F:96:PRO:HB3	18:R:30:ASP:CG	2.32	0.49
17:Q:55:ASP:HA	17:Q:79:SER:HA	1.94	0.49
9:I:21:PRO:HA	9:I:59:PHE:HD1	1.76	0.49
20:T:56:MET:HE1	20:T:85:MET:HG2	1.93	0.49
7:G:130:GLY:HA2	7:G:135:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:167:PRO:HD3	2:B:187:LEU:O	2.12	0.49
1:A:951:G:H4'	1:A:972:C:H5	1.78	0.49
11:K:69:ALA:HB1	11:K:103:LEU:HD21	1.94	0.49
1:A:977:A:H2'	1:A:977:A:N3	2.27	0.49
3:C:73:PRO:HB3	3:C:103:VAL:HG11	1.94	0.49
19:S:50:ALA:CB	19:S:57:HIS:HB3	2.43	0.49
1:A:1143:G:H2'	1:A:1144:G:C8	2.47	0.49
1:A:544:G:OP1	4:D:62:GLN:NE2	2.23	0.49
20:T:77:ALA:O	20:T:81:LYS:HG3	2.13	0.49
1:A:532:A:H61	3:C:193:TYR:HB3	1.78	0.49
3:C:192:THR:OG1	3:C:193:TYR:N	2.43	0.49
3:C:138:VAL:HG22	3:C:149:ALA:HB1	1.95	0.49
5:E:107:ARG:O	5:E:110:LEU:N	2.45	0.49
8:H:57:PRO:O	8:H:58:TYR:HD1	1.95	0.49
6:F:91:VAL:CG1	18:R:72:ARG:HH12	2.26	0.49
1:A:429:U:C3'	4:D:22:LYS:HZ3	2.25	0.49
1:A:1115:C:O2	1:A:1185:G:N1	2.35	0.49
1:A:920:U:C2	1:A:921:U:C5	3.01	0.49
3:C:131:ARG:HH22	5:E:50:GLU:CD	2.16	0.49
3:C:142:MET:HA	3:C:146:ALA:HB3	1.95	0.49
1:A:1135:U:O2'	1:A:1137:C:H5'	2.12	0.49
20:T:41:ILE:HG22	20:T:91:LEU:HD12	1.93	0.49
1:A:728:A:H2'	1:A:729:A:C8	2.47	0.49
2:B:32:ILE:HD11	2:B:190:THR:HG22	1.94	0.49
2:B:204:ASN:CG	2:B:206:ASP:H	2.15	0.49
1:A:1025:U:O2	1:A:1036:G:C6	2.66	0.49
1:A:994:A:H2	14:N:4:LYS:HD2	1.78	0.49
1:A:557:G:C6	1:A:558:G:C6	3.01	0.49
9:I:40:LEU:HD11	9:I:70:LYS:HB3	1.95	0.49
1:A:626:U:H5''	16:P:38:TYR:CD2	2.48	0.49
13:M:59:TYR:CZ	13:M:63:THR:HG21	2.47	0.49
1:A:169:C:H5	1:A:170:U:C4	2.31	0.49
5:E:53:LEU:O	5:E:56:GLN:HB3	2.13	0.49
1:A:1003:G:N2	1:A:1037:C:C2	2.80	0.49
1:A:1003:G:C2	1:A:1037:C:N3	2.81	0.49
1:A:1360:A:N7	14:N:18:VAL:HG13	2.27	0.49
1:A:590:C:H2'	1:A:591:U:C6	2.45	0.49
1:A:35:G:C6	1:A:36:C:N4	2.81	0.49
2:B:61:LEU:HD21	2:B:160:ASP:HB2	1.94	0.49
1:A:1369:C:H2'	1:A:1370:G:C8	2.47	0.49
1:A:414:A:C5	1:A:431:A:C2	3.01	0.49
3:C:54:ARG:HG2	3:C:56:ASP:H	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:11:PHE:HE2	10:J:67:THR:HB	1.77	0.49
1:A:499:A:H4'	1:A:500:G:OP1	2.12	0.49
1:A:1269:A:C8	1:A:1270:C:H1'	2.48	0.49
2:B:102:LEU:O	2:B:105:PHE:HB2	2.13	0.49
10:J:81:THR:O	10:J:85:LEU:N	2.44	0.49
1:A:918:A:H2'	1:A:919:A:C8	2.48	0.49
4:D:148:VAL:HG12	4:D:149:ALA:H	1.77	0.49
1:A:937:A:H1'	1:A:1379:G:N2	2.28	0.49
1:A:39:G:N7	1:A:547:A:H8	2.10	0.49
1:A:1118:C:H2'	1:A:1119:C:C5	2.47	0.49
2:B:21:ARG:HH12	2:B:23:ARG:HE	1.59	0.49
1:A:375:U:H2'	1:A:376:G:H8	1.78	0.49
2:B:224:GLN:OE1	2:B:225:ALA:N	2.46	0.49
1:A:1490:C:H2'	1:A:1491:G:O4'	2.13	0.49
1:A:1288:A:H2'	1:A:1289:A:O4'	2.13	0.48
1:A:1138:G:C6	1:A:1140:C:H1'	2.48	0.48
3:C:152:ILE:HG22	3:C:166:GLU:O	2.13	0.48
1:A:1012:U:H3'	1:A:1013:G:C8	2.47	0.48
1:A:36:C:H5''	12:L:123:LYS:HD3	1.94	0.48
1:A:1378:C:H3'	1:A:1379:G:H5''	1.95	0.48
1:A:1168:A:C2	1:A:1169:A:C4	3.01	0.48
6:F:41:GLU:O	6:F:43:LEU:HD12	2.13	0.48
1:A:1170:A:N6	1:A:1171:G:C2	2.81	0.48
1:A:1360:A:H8	1:A:1360:A:OP1	1.96	0.48
1:A:1057:G:H5'	3:C:155:GLY:HA2	1.95	0.48
1:A:502:G:C2	1:A:503:C:C2	3.01	0.48
2:B:87:ARG:HG3	2:B:233:SER:OG	2.13	0.48
7:G:14:PRO:HG3	7:G:21:VAL:HG12	1.94	0.48
1:A:1186:G:C2	1:A:1187:G:H1'	2.47	0.48
9:I:26:VAL:HA	9:I:61:ALA:HB3	1.95	0.48
12:L:76:ASN:HD21	12:L:107:ALA:HA	1.79	0.48
1:A:1299:A:H2'	1:A:1301:U:C6	2.48	0.48
4:D:134:ASP:O	4:D:136:PRO:HD3	2.14	0.48
14:N:47:LEU:HA	14:N:50:LYS:HB2	1.95	0.48
20:T:42:GLN:NE2	20:T:42:GLN:HA	2.28	0.48
2:B:82:ARG:HG3	2:B:92:TYR:CZ	2.48	0.48
4:D:14:ARG:HG3	4:D:59:ARG:HH21	1.79	0.48
4:D:127:THR:OG1	4:D:128:VAL:N	2.46	0.48
4:D:173:TRP:NE1	4:D:174:LEU:HG	2.29	0.48
1:A:618:C:N4	1:A:621:A:N7	2.60	0.48
19:S:22:LEU:O	19:S:27:GLU:HA	2.13	0.48
5:E:67:VAL:HG21	5:E:140:ARG:HA	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:170:GLU:O	2:B:173:ALA:N	2.46	0.48
4:D:68:TYR:CE2	4:D:97:LEU:HD22	2.49	0.48
17:Q:22:LEU:HD13	17:Q:41:LYS:HG2	1.95	0.48
1:A:1095:U:H2'	1:A:1096:C:N1	2.28	0.48
1:A:983:A:H2	1:A:984:C:C6	2.32	0.48
1:A:669:U:H2'	1:A:670:G:C8	2.48	0.48
1:A:102:G:H2'	1:A:103:C:H6	1.79	0.48
1:A:170:U:O2'	1:A:171:A:H5'	2.14	0.48
11:K:21:ILE:HG12	11:K:30:VAL:HG12	1.95	0.48
12:L:42:THR:OG1	12:L:52:LEU:HD12	2.14	0.48
15:O:55:GLY:HA2	15:O:58:MET:HG3	1.96	0.48
1:A:1442:G:C8	1:A:1442(A):G:C5	3.02	0.48
13:M:102:ARG:HE	13:M:104:ARG:HB3	1.79	0.48
1:A:154:C:C2	1:A:168:G:C2	3.02	0.48
1:A:1192:C:N4	1:A:1193:G:C4	2.81	0.48
1:A:745:C:H2'	1:A:746:A:C8	2.49	0.48
1:A:1346:A:N1	1:A:1374:A:H5''	2.28	0.48
1:A:1370:G:C8	9:I:109:VAL:HG21	2.49	0.48
1:A:1308:U:OP1	13:M:98:VAL:HG23	2.13	0.48
1:A:359:U:H2'	1:A:360:A:C8	2.48	0.48
1:A:1022:G:H2'	1:A:1023:G:C8	2.49	0.48
1:A:1349:A:C2	1:A:1350:A:H1'	2.49	0.48
1:A:1286:A:H61	1:A:1355:G:P	2.37	0.48
1:A:1321:C:H5'	1:A:1322:C:H5''	1.96	0.48
1:A:447:G:H2'	1:A:485:G:N2	2.29	0.48
1:A:1329:A:H4'	13:M:24:GLY:HA2	1.96	0.48
7:G:85:TYR:CD1	7:G:154:TYR:HE1	2.32	0.48
16:P:72:ARG:HG2	16:P:73:LEU:HD23	1.96	0.48
1:A:801:U:H2'	1:A:802:A:C8	2.49	0.48
3:C:181:ASN:OD1	3:C:204:LEU:HB2	2.13	0.48
1:A:1203:C:H2'	1:A:1204:A:C8	2.49	0.48
1:A:433:C:H2'	1:A:434:U:H6	1.78	0.48
1:A:176:C:H2'	1:A:177:C:H6	1.79	0.48
4:D:101:LEU:HD23	4:D:121:VAL:HG11	1.94	0.48
5:E:32:VAL:HB	5:E:58:ALA:HB1	1.95	0.48
1:A:441:A:H3'	1:A:442:C:C6	2.49	0.48
1:A:1325:C:H5''	21:U:17:THR:HG21	1.96	0.48
1:A:148:G:O2'	1:A:149:A:H5'	2.13	0.48
1:A:1403:C:H1'	1:A:1500:A:N1	2.29	0.48
1:A:980:C:H3'	1:A:981:U:C6	2.49	0.48
20:T:76:ALA:HA	20:T:79:ARG:NH1	2.29	0.48
3:C:175:LEU:HG	3:C:175:LEU:H	1.54	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:G:C6	1:A:93:G:C6	3.02	0.48
7:G:92:SER:HB3	7:G:95:ARG:HB3	1.95	0.47
1:A:1131:G:N2	1:A:1143:G:O2'	2.46	0.47
19:S:37:ARG:O	19:S:70:LYS:HE3	2.14	0.47
1:A:1126:U:OP2	1:A:1281:U:H1'	2.14	0.47
1:A:949:A:H2	1:A:971:G:N7	2.12	0.47
1:A:589:C:H2'	1:A:590:C:C6	2.49	0.47
10:J:8:LEU:HD22	10:J:96:ILE:HG22	1.95	0.47
1:A:202:U:H3'	1:A:203:U:C5	2.49	0.47
5:E:127:ASN:O	5:E:131:ILE:HG12	2.14	0.47
1:A:1081:G:H2'	1:A:1082:G:O4'	2.14	0.47
7:G:143:ARG:CZ	7:G:143:ARG:HB2	2.44	0.47
1:A:1459:C:C2	1:A:1460:A:N6	2.83	0.47
1:A:1244:C:H2'	1:A:1245:A:H8	1.75	0.47
7:G:116:ALA:HA	7:G:119:ARG:CG	2.44	0.47
1:A:1055:A:N1	1:A:1056:U:H1'	2.29	0.47
1:A:722:A:O2'	1:A:723:U:H5"	2.14	0.47
7:G:104:LEU:HD22	7:G:134:ALA:HB1	1.97	0.47
1:A:1286:A:H2'	1:A:1287:A:H4'	1.96	0.47
1:A:1273:G:N3	1:A:1273:G:H2'	2.28	0.47
1:A:1138:G:N3	1:A:1138:G:H3'	2.30	0.47
13:M:92:HIS:CD2	13:M:98:VAL:HG21	2.50	0.47
1:A:1128:C:OP1	9:I:66:ARG:NH2	2.48	0.47
1:A:1411:C:H2'	1:A:1412:C:C6	2.49	0.47
1:A:203:U:OP2	1:A:203:U:H3'	2.14	0.47
1:A:577:G:C8	1:A:816:A:C6	3.03	0.47
20:T:30:LYS:HA	20:T:33:ILE:HD12	1.95	0.47
3:C:131:ARG:NH2	5:E:50:GLU:OE1	2.45	0.47
1:A:715:A:H2'	1:A:716:A:C8	2.48	0.47
9:I:113:LYS:HB2	9:I:119:ALA:HA	1.96	0.47
5:E:76:ILE:HG22	5:E:93:PRO:HB3	1.97	0.47
5:E:93:PRO:HG2	8:H:105:ARG:CZ	2.45	0.47
1:A:547:A:OP2	4:D:2:GLY:HA2	2.13	0.47
1:A:1127:G:H4'	9:I:66:ARG:HH12	1.79	0.47
7:G:26:PHE:CD1	7:G:101:LEU:HB3	2.47	0.47
7:G:26:PHE:HE1	7:G:101:LEU:O	1.97	0.47
3:C:191:THR:OG1	3:C:192:THR:N	2.46	0.47
1:A:920:U:H2'	1:A:921:U:H6	1.79	0.47
17:Q:51:TYR:HE2	17:Q:76:LEU:HB2	1.80	0.47
1:A:1290:G:C6	1:A:1291:G:C6	3.03	0.47
1:A:1306:A:H2'	1:A:1307:U:C6	2.49	0.47
1:A:1396:A:H2	5:E:19:MET:HG3	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1065:U:O2'	1:A:1066:C:OP2	2.21	0.47
4:D:88:VAL:O	4:D:92:VAL:HG23	2.14	0.47
1:A:580:U:H3	1:A:761:G:H1	1.62	0.47
1:A:493:G:HO2'	1:A:494:U:H6	1.60	0.47
1:A:1035:A:H2'	1:A:1036:G:C8	2.48	0.47
1:A:1373:G:C5'	7:G:36:LYS:HB2	2.42	0.47
1:A:426:G:P	4:D:36:ARG:NH1	2.87	0.47
1:A:1096:C:H2'	1:A:1097:C:C6	2.47	0.47
1:A:59:A:H5'	1:A:60:A:C5'	2.44	0.47
1:A:939:G:H1	1:A:1344:C:N4	2.12	0.47
1:A:397:A:H5''	1:A:397:A:N3	2.29	0.47
1:A:622:A:OP2	1:A:623:C:N4	2.47	0.47
1:A:438:G:OP1	4:D:125:HIS:CE1	2.66	0.47
1:A:266:G:H5''	1:A:267:C:H5	1.79	0.47
1:A:745:C:OP1	1:A:851:G:O2'	2.27	0.47
12:L:57:LYS:HE2	12:L:67:THR:HG23	1.97	0.47
12:L:5:PRO:HB2	12:L:10:LEU:HD11	1.96	0.47
3:C:117:ALA:HB2	3:C:200:ALA:HB2	1.97	0.47
15:O:24:SER:O	15:O:27:VAL:N	2.47	0.47
1:A:1171:G:H2'	1:A:1172:C:C6	2.50	0.47
1:A:1236:A:O3'	1:A:1304:G:H5'	2.13	0.47
19:S:52:TYR:HD1	19:S:57:HIS:CD2	2.32	0.47
2:B:71:VAL:HG13	2:B:93:VAL:HG23	1.95	0.47
1:A:408:A:H61	1:A:434:U:H3	1.62	0.47
13:M:97:PRO:HB3	13:M:101:GLN:CD	2.36	0.47
1:A:44:G:H2'	1:A:45:U:O4'	2.15	0.47
3:C:9:GLY:HA3	14:N:49:HIS:ND1	2.30	0.47
4:D:64:LEU:HD23	4:D:203:VAL:HG21	1.96	0.47
1:A:78:G:N2	1:A:92:C:O2	2.48	0.47
6:F:15:ASP:HB2	6:F:18:GLN:H	1.79	0.47
20:T:73:HIS:C	20:T:74:LYS:HG2	2.36	0.47
15:O:56:LEU:O	15:O:60:VAL:HG23	2.15	0.47
20:T:55:ILE:HD13	20:T:55:ILE:HA	1.77	0.47
1:A:1356:G:H2'	1:A:1357:A:O4'	2.15	0.47
1:A:1319:A:H2'	19:S:4:SER:HB2	1.97	0.47
1:A:1347:G:N2	1:A:1373:G:H2'	2.30	0.47
1:A:1015:A:H2'	1:A:1016:A:O4'	2.15	0.47
1:A:509:A:H5''	4:D:55:ALA:HB2	1.95	0.47
13:M:91:ARG:HG3	13:M:98:VAL:HA	1.97	0.47
2:B:21:ARG:N	2:B:21:ARG:HD3	2.29	0.47
5:E:59:GLY:O	5:E:63:ARG:N	2.42	0.47
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1236:A:OP1	21:U:2:GLY:HA3	2.15	0.46
4:D:36:ARG:HG2	4:D:38:TYR:CZ	2.51	0.46
4:D:36:ARG:HG2	4:D:38:TYR:OH	2.15	0.46
4:D:119:GLN:O	4:D:123:HIS:CD2	2.69	0.46
1:A:978:A:H5''	1:A:979:C:OP2	2.14	0.46
4:D:120:LEU:HB3	4:D:126:ILE:HD11	1.95	0.46
2:B:134:GLU:O	2:B:138:LEU:HG	2.14	0.46
1:A:1233:G:H2'	1:A:1234:C:C6	2.50	0.46
1:A:622:A:C8	1:A:623:C:C6	3.03	0.46
3:C:184:TYR:CE2	3:C:186:PHE:HB2	2.50	0.46
1:A:152:A:N6	1:A:170:U:H3	2.12	0.46
1:A:1252:A:H2'	1:A:1253:G:O4'	2.16	0.46
1:A:31:G:O2'	1:A:48:C:N4	2.48	0.46
1:A:509:A:H3'	1:A:509:A:H8	1.80	0.46
1:A:1459:C:C4	1:A:1460:A:N6	2.73	0.46
1:A:662:G:O2'	1:A:836:G:OP1	2.32	0.46
6:F:8:ILE:HD12	6:F:26:ILE:HD13	1.97	0.46
1:A:937:A:H1'	1:A:1379:G:H22	1.81	0.46
2:B:113:HIS:O	2:B:117:GLU:HG3	2.16	0.46
1:A:1459:C:H2'	1:A:1460:A:C8	2.50	0.46
1:A:1085:U:H3'	1:A:1086:U:H5	1.80	0.46
1:A:865:A:H5'	1:A:1078:U:O4	2.15	0.46
1:A:376:G:P	16:P:67:THR:HG21	2.55	0.46
5:E:137:GLU:O	5:E:141:GLN:HG3	2.15	0.46
1:A:1369:C:OP2	9:I:112:LYS:N	2.37	0.46
16:P:28:ARG:HG2	16:P:29:ASP:OD2	2.16	0.46
13:M:23:TYR:HE1	13:M:70:LEU:HD21	1.79	0.46
1:A:79:G:H2'	1:A:80:G:C8	2.50	0.46
1:A:186:C:H2'	1:A:187:C:H6	1.79	0.46
8:H:120:THR:H	8:H:123:GLU:HB2	1.80	0.46
20:T:79:ARG:HD2	20:T:83:ARG:HH21	1.80	0.46
12:L:102:ARG:HE	12:L:102:ARG:HB3	1.44	0.46
1:A:719:C:H5	1:A:720:C:C4	2.33	0.46
1:A:517:G:N2	1:A:531:U:H5'	2.31	0.46
1:A:115:G:H4'	1:A:116:A:O5'	2.15	0.46
2:B:75:LYS:HE3	2:B:78:GLN:OE1	2.16	0.46
1:A:1273:G:H5'	1:A:1274:G:OP2	2.16	0.46
15:O:63:ARG:HG2	15:O:67:LEU:HD12	1.97	0.46
1:A:544:G:C2	1:A:545:C:C2	3.04	0.46
7:G:87:VAL:HG11	7:G:155:ARG:HB2	1.96	0.46
1:A:1246:C:H2'	1:A:1247:U:O4'	2.15	0.46
1:A:1184:G:N3	1:A:1184:G:H2'	2.30	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1512:U:H2'	1:A:1513:A:C8	2.50	0.46
9:I:49:PRO:HG3	9:I:101:PHE:CG	2.51	0.46
2:B:149:LEU:HD22	2:B:152:PHE:CD1	2.50	0.46
1:A:745:C:H2'	1:A:746:A:H8	1.80	0.46
1:A:93:G:H1'	1:A:96:U:H5'	1.97	0.46
10:J:34:VAL:HG12	10:J:74:ILE:HA	1.97	0.46
11:K:122:LYS:HE2	11:K:122:LYS:HB3	1.68	0.46
1:A:373:A:N3	1:A:481:G:N2	2.51	0.46
1:A:1122:U:O4	1:A:1123:A:N6	2.47	0.46
4:D:104:VAL:HA	4:D:107:ARG:HB2	1.97	0.46
1:A:658:G:H2'	1:A:659:U:H6	1.81	0.46
1:A:1060:C:OP1	10:J:51:ARG:NH1	2.48	0.46
9:I:33:PHE:O	9:I:37:PHE:HB2	2.16	0.46
1:A:344:A:H3'	1:A:346:G:O6	2.16	0.46
1:A:1236:A:H2'	1:A:1237:C:C6	2.51	0.46
1:A:1360:A:C8	14:N:18:VAL:HG22	2.50	0.46
1:A:353:A:H5'	1:A:353:A:C8	2.42	0.46
1:A:658:G:C4	1:A:659:U:C5	3.04	0.46
1:A:479:C:H2'	1:A:480:U:H6	1.80	0.46
7:G:36:LYS:HA	7:G:36:LYS:HD3	1.80	0.46
18:R:31:LEU:H	18:R:31:LEU:CD2	2.29	0.46
1:A:626:U:H5''	16:P:38:TYR:CG	2.51	0.46
1:A:980:C:H3'	1:A:981:U:H6	1.81	0.46
1:A:1007:C:H2'	1:A:1008:C:C6	2.51	0.46
4:D:111:ALA:HB1	4:D:116:GLN:HG2	1.98	0.46
19:S:36:ARG:HB3	19:S:72:GLY:HA3	1.98	0.46
1:A:599:C:H5''	8:H:95:VAL:O	2.15	0.46
1:A:589:C:H2'	1:A:590:C:H6	1.81	0.46
1:A:1250:A:H4'	9:I:67:GLY:HA2	1.96	0.46
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.98	0.46
2:B:73:THR:HG21	2:B:95:GLN:O	2.16	0.46
1:A:1531:A:H2'	1:A:1532:U:O4'	2.16	0.46
1:A:511:C:N3	1:A:540:G:N2	2.54	0.45
8:H:86:ILE:HG21	8:H:133:LEU:HD22	1.98	0.45
1:A:1227:A:OP2	13:M:111:LYS:HG2	2.16	0.45
12:L:60:LEU:H	12:L:60:LEU:HD22	1.80	0.45
2:B:47:THR:O	2:B:51:LEU:HB2	2.16	0.45
5:E:133:TYR:O	5:E:137:GLU:HB2	2.15	0.45
5:E:151:LEU:HB3	8:H:79:VAL:HG22	1.98	0.45
1:A:791:G:C6	1:A:792:A:N7	2.83	0.45
4:D:25:ARG:O	4:D:25:ARG:HG2	2.16	0.45
1:A:1347:G:H8	9:I:107:ARG:CB	2.26	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:59:ARG:HA	4:D:59:ARG:HH11	1.81	0.45
2:B:187:LEU:HA	2:B:201:ILE:HB	1.98	0.45
1:A:674:G:H2'	1:A:675:A:C8	2.47	0.45
3:C:150:LYS:HB3	3:C:150:LYS:NZ	2.31	0.45
1:A:874:G:C6	1:A:875:C:C4	3.04	0.45
1:A:623:C:H2'	1:A:624:C:C6	2.48	0.45
1:A:475:G:H2'	1:A:476:G:C8	2.49	0.45
7:G:112:PRO:O	7:G:119:ARG:HD3	2.16	0.45
1:A:1067:A:O2'	1:A:1068:G:OP2	2.26	0.45
6:F:33:TYR:HB2	6:F:75:LEU:HD12	1.97	0.45
3:C:23:TYR:OH	3:C:25:GLY:HA3	2.17	0.45
11:K:16:SER:HA	11:K:79:SER:HB3	1.98	0.45
2:B:219:VAL:O	2:B:222:ILE:HB	2.16	0.45
1:A:441:A:H3'	1:A:442:C:H6	1.81	0.45
2:B:59:GLU:O	2:B:63:MET:HG2	2.16	0.45
1:A:988:G:H2'	1:A:989:C:O4'	2.16	0.45
2:B:194:PRO:O	2:B:196:LEU:N	2.48	0.45
1:A:491:G:C4	1:A:492:G:C8	3.04	0.45
1:A:1002:G:C2	1:A:1003:G:H1'	2.51	0.45
7:G:87:VAL:HG13	7:G:151:TYR:HB2	1.99	0.45
2:B:136:VAL:HA	2:B:139:LYS:CG	2.43	0.45
1:A:1155:G:H2'	1:A:1156:G:C8	2.51	0.45
1:A:1302:U:C5	13:M:17:VAL:HG21	2.51	0.45
1:A:1233:G:H2'	1:A:1234:C:H6	1.81	0.45
5:E:57:LYS:HB3	5:E:61:TYR:CE2	2.50	0.45
11:K:29:ILE:HG23	11:K:44:SER:HB3	1.99	0.45
1:A:426:G:H2'	1:A:427:U:C6	2.52	0.45
4:D:59:ARG:NH1	4:D:59:ARG:HA	2.31	0.45
1:A:1179:A:H8	1:A:1179:A:OP1	1.99	0.45
8:H:9:MET:O	8:H:12:ARG:N	2.49	0.45
20:T:64:ASP:OD1	20:T:81:LYS:NZ	2.47	0.45
1:A:35:G:N2	1:A:550:G:N3	2.65	0.45
1:A:801:U:H2'	1:A:802:A:H8	1.82	0.45
1:A:1002:G:N2	1:A:1003:G:H1'	2.31	0.45
1:A:1137:C:H4'	1:A:1138:G:C2	2.52	0.45
1:A:1399:C:C2	1:A:1502:A:N6	2.85	0.45
1:A:1441:G:H21	1:A:1459:C:H6	1.64	0.45
1:A:952:U:H4'	1:A:964:A:N1	2.32	0.45
4:D:61:LYS:O	4:D:65:ARG:HB2	2.17	0.45
16:P:43:LYS:HG2	16:P:48:TRP:CE3	2.52	0.45
20:T:29:LYS:O	20:T:33:ILE:HG13	2.17	0.45
1:A:1250:A:O3'	9:I:67:GLY:HA2	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1491:G:H5''	1:A:1492:A:OP2	2.16	0.45
1:A:714:G:H2'	1:A:715:A:C8	2.51	0.45
1:A:116:A:H61	1:A:313:A:H1'	1.82	0.45
15:O:7:GLU:O	15:O:10:LYS:HB3	2.16	0.45
1:A:573:A:N3	1:A:883:C:O2'	2.41	0.45
1:A:298:A:OP1	1:A:298:A:H8	2.00	0.45
9:I:16:ARG:HB2	9:I:64:THR:HG23	1.98	0.45
1:A:328:C:H4'	1:A:329:A:H5'	1.98	0.45
7:G:146:GLU:HA	7:G:149:ARG:HB2	1.98	0.45
1:A:426:G:P	4:D:36:ARG:HH12	2.40	0.45
18:R:59:SER:OG	18:R:60:ALA:N	2.50	0.45
12:L:67:THR:OG1	12:L:95:GLY:O	2.31	0.45
1:A:57:G:H2'	1:A:58:C:C6	2.52	0.45
1:A:530:G:H3'	1:A:530:G:OP1	2.17	0.45
1:A:405:U:H3'	1:A:406:G:H5'	1.97	0.45
1:A:956:U:H1'	1:A:1225:A:H2	1.81	0.45
1:A:154:C:C4	1:A:168:G:N1	2.84	0.45
2:B:87:ARG:CZ	2:B:233:SER:HB2	2.46	0.45
1:A:77:G:C6	1:A:78:G:C6	3.04	0.45
1:A:505:G:C6	1:A:535:A:C2	3.05	0.45
12:L:47:LYS:HA	12:L:49:ASN:H	1.82	0.45
11:K:66:LEU:HD21	11:K:97:ALA:HB1	1.98	0.45
1:A:994:A:N3	1:A:994:A:H2'	2.31	0.45
1:A:1342:C:H1'	9:I:124:GLN:NE2	2.32	0.45
6:F:11:ASN:HA	6:F:12:PRO:HD2	1.63	0.45
3:C:34:LEU:O	3:C:38:ARG:HG3	2.17	0.45
1:A:600:C:H2'	1:A:601:C:H6	1.81	0.45
8:H:9:MET:SD	8:H:32:LYS:HG2	2.57	0.45
3:C:156:ARG:HD3	3:C:193:TYR:HB2	1.99	0.45
1:A:688:G:O2'	1:A:704:A:N1	2.43	0.45
18:R:61:LYS:O	18:R:65:ILE:HG12	2.17	0.45
1:A:717:C:H6	1:A:717:C:H5''	1.81	0.45
1:A:1002:G:C2	1:A:1039:C:C2	3.05	0.44
1:A:1156:G:H2'	1:A:1157:A:H5''	1.99	0.44
8:H:9:MET:HG3	8:H:26:VAL:HG11	1.99	0.44
1:A:1327:C:H2'	1:A:1328:C:C6	2.52	0.44
1:A:728:A:H2'	1:A:729:A:H8	1.81	0.44
5:E:50:GLU:HB2	5:E:53:LEU:HD13	1.99	0.44
2:B:204:ASN:OD1	2:B:206:ASP:N	2.46	0.44
1:A:1034:G:N2	1:A:1035:A:N6	2.65	0.44
1:A:1030:C:N4	1:A:1032:G:C4	2.85	0.44
5:E:7:GLU:HG2	5:E:112:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:29:LYS:HZ1	7:G:102:ARG:HE	1.65	0.44
22:V:30:PRO:HB3	22:V:40:TRP:CE2	2.51	0.44
1:A:1371:G:H5''	9:I:68:GLY:HA2	2.00	0.44
1:A:943:U:H2'	1:A:944:G:H8	1.83	0.44
10:J:49:VAL:HG21	14:N:45:ARG:CD	2.44	0.44
1:A:1097:C:H2'	1:A:1098:C:O4'	2.17	0.44
1:A:503:C:H2'	1:A:504:C:H6	1.83	0.44
10:J:54:PHE:CE2	10:J:55:LYS:HG3	2.52	0.44
8:H:73:ASP:HA	8:H:74:PRO:HD2	1.75	0.44
7:G:80:VAL:HG12	7:G:80:VAL:O	2.18	0.44
1:A:474:G:H2'	1:A:475:G:H8	1.81	0.44
1:A:1151:A:C2	10:J:39:PRO:HG2	2.52	0.44
1:A:192:U:H2'	1:A:193:C:H6	1.82	0.44
1:A:1531:A:H5'	25:A:1773:HOH:O	2.16	0.44
1:A:790:A:C6	1:A:791:G:C6	3.05	0.44
1:A:1424:C:H2'	1:A:1425:U:O4'	2.17	0.44
17:Q:48:GLU:HG3	17:Q:50:LYS:HE3	2.00	0.44
8:H:112:LEU:HB3	8:H:133:LEU:HA	1.99	0.44
3:C:118:GLN:HB3	3:C:118:GLN:HE21	1.63	0.44
13:M:23:TYR:O	13:M:66:LEU:HA	2.17	0.44
1:A:165:C:H2'	1:A:166:G:H8	1.83	0.44
1:A:1492:A:OP1	1:A:1492:A:H4'	2.18	0.44
3:C:182:ILE:HG23	3:C:203:PHE:HB2	1.99	0.44
9:I:44:VAL:HA	9:I:45:ALA:HA	1.68	0.44
1:A:633:G:C5	1:A:634:C:C4	3.06	0.44
1:A:189:G:C6	1:A:189(A):C:C4	3.05	0.44
1:A:657:G:C2	1:A:750:G:C5	3.04	0.44
1:A:750:G:N3	15:O:23:GLY:HA3	2.32	0.44
4:D:166:LYS:HA	4:D:178:VAL:HG11	1.99	0.44
1:A:540:G:H2'	1:A:541:G:O4'	2.18	0.44
1:A:1459:C:H2'	1:A:1460:A:N7	2.33	0.44
1:A:586:C:O2'	1:A:878:G:H4'	2.17	0.44
1:A:827:U:H5''	1:A:828:A:OP2	2.17	0.44
1:A:921:U:H2'	1:A:922:G:O4'	2.17	0.44
12:L:41:ARG:HH12	12:L:57:LYS:HE3	1.82	0.44
12:L:124:LYS:HA	12:L:125:PRO:HD3	1.76	0.44
1:A:1003:G:N2	1:A:1038:C:N3	2.65	0.44
1:A:1288:A:C6	1:A:1289:A:C5	3.05	0.44
8:H:40:ALA:HA	8:H:45:ILE:HG13	1.99	0.44
7:G:48:LYS:HA	7:G:51:GLN:HB2	1.99	0.44
1:A:869:G:H4'	1:A:872:A:O4'	2.17	0.44
1:A:324:G:N2	1:A:327:A:C8	2.86	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1190:G:P	3:C:5:ILE:HG22	2.57	0.44
1:A:69:G:N1	1:A:70:G:C5	2.86	0.44
4:D:200:GLU:O	4:D:204:ILE:HG12	2.17	0.44
16:P:71:ARG:HA	16:P:74:LEU:HB2	2.00	0.44
19:S:63:THR:HB	19:S:65:ASN:H	1.82	0.44
1:A:1102:A:C5	1:A:1103:C:C5	3.05	0.44
7:G:64:GLN:HE22	7:G:67:GLU:HB3	1.81	0.44
6:F:25:ILE:CD1	6:F:82:ARG:HE	2.31	0.44
1:A:1373:G:H5'	7:G:36:LYS:HE2	1.99	0.44
4:D:128:VAL:CG1	4:D:129:ASN:HD22	2.22	0.44
1:A:521:G:OP1	12:L:73:GLU:HA	2.17	0.44
1:A:969:A:H2'	1:A:970:C:O4'	2.17	0.44
9:I:28:VAL:HG22	9:I:63:ILE:HD12	2.00	0.44
1:A:1206:G:C6	1:A:1207:G:C5	3.06	0.44
1:A:185:A:H2'	1:A:186:C:C6	2.53	0.44
17:Q:81:ARG:HD2	17:Q:81:ARG:HA	1.63	0.44
1:A:881:G:P	12:L:12:ARG:NH2	2.89	0.44
1:A:858:G:O6	1:A:869:G:H3'	2.18	0.44
1:A:270:A:H2'	1:A:271:C:C6	2.53	0.44
1:A:1300:G:HO2'	1:A:1301:U:P	2.41	0.44
5:E:110:LEU:HD12	5:E:118:ILE:HG21	1.99	0.44
1:A:1492:A:H2'	1:A:1492:A:N3	2.32	0.44
2:B:75:LYS:HA	2:B:78:GLN:HB2	2.00	0.44
2:B:27:LYS:HB3	2:B:194:PRO:HD2	2.00	0.44
18:R:43:PHE:C	18:R:51:LEU:HD12	2.38	0.44
16:P:76:GLN:O	16:P:76:GLN:HG3	2.18	0.44
5:E:29:GLY:HA2	5:E:47:LYS:HA	1.99	0.44
1:A:1150:U:H1'	1:A:1280:A:C6	2.52	0.44
1:A:1127:G:C4	1:A:1147:C:N4	2.86	0.44
1:A:433:C:H2'	1:A:434:U:C6	2.53	0.44
1:A:99:U:H2'	1:A:100:C:H6	1.82	0.44
4:D:50:ARG:HA	4:D:51:PRO:HD3	1.86	0.44
3:C:123:GLN:HA	3:C:126:ARG:HH11	1.81	0.44
1:A:1340:A:C2'	1:A:1341:U:H5'	2.48	0.44
1:A:355:C:C4	1:A:356:A:N7	2.86	0.44
1:A:1001(A):G:H2'	1:A:1002:G:C8	2.50	0.43
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.81	0.43
7:G:92:SER:H	7:G:95:ARG:HD3	1.83	0.43
1:A:1014:A:C2	1:A:1219:U:H1'	2.53	0.43
8:H:92:ARG:HD3	8:H:92:ARG:HA	1.74	0.43
1:A:458:C:H2'	1:A:460:G:C8	2.50	0.43
13:M:43:THR:OG1	13:M:47:ASP:O	2.36	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:872:A:C5	1:A:874:G:C8	3.06	0.43
1:A:152:A:N6	1:A:170:U:N3	2.66	0.43
1:A:1468:A:H2'	1:A:1469:G:O4'	2.18	0.43
1:A:966:G:H2'	1:A:967:C:O4'	2.18	0.43
1:A:990:C:H2'	1:A:991:U:C6	2.53	0.43
1:A:832:C:N4	1:A:855:G:C6	2.85	0.43
1:A:1013:G:H1'	1:A:1017:G:H1	1.82	0.43
1:A:1310:G:H1	1:A:1327:C:N4	2.16	0.43
2:B:40:HIS:HB3	2:B:190:THR:HG21	1.98	0.43
16:P:39:TYR:CD1	16:P:73:LEU:HD13	2.53	0.43
1:A:114:U:H2'	1:A:115:G:C8	2.53	0.43
7:G:146:GLU:HG2	7:G:149:ARG:HG3	2.00	0.43
12:L:48:PRO:C	12:L:49:ASN:HD22	2.21	0.43
1:A:507:C:OP2	1:A:508:C:O2'	2.28	0.43
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.53	0.43
12:L:54:LYS:HB3	12:L:70:ILE:HD12	1.99	0.43
1:A:568:G:C6	1:A:569:C:N4	2.86	0.43
1:A:345:C:H4'	1:A:346:G:N7	2.32	0.43
2:B:139:LYS:O	2:B:143:GLU:HB2	2.18	0.43
4:D:107:ARG:O	4:D:170:VAL:HG11	2.18	0.43
2:B:71:VAL:N	2:B:163:PHE:O	2.46	0.43
3:C:177:THR:HG22	3:C:179:ARG:H	1.82	0.43
1:A:1308:U:O2'	1:A:1309:G:H5'	2.19	0.43
1:A:1234:C:H2'	1:A:1235:U:C6	2.54	0.43
1:A:832:C:O2'	1:A:833:U:P	2.76	0.43
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.89	0.43
1:A:865:A:C2	1:A:918:A:H4'	2.53	0.43
1:A:750:G:H1'	15:O:22:THR:OG1	2.19	0.43
16:P:55:ARG:O	16:P:58:TYR:N	2.51	0.43
7:G:150:ALA:HB2	11:K:50:TYR:OH	2.18	0.43
14:N:13:THR:HA	14:N:14:PRO:HD2	1.88	0.43
16:P:54:GLU:H	16:P:54:GLU:HG2	1.45	0.43
1:A:1315:U:H2'	1:A:1316:G:O4'	2.18	0.43
1:A:1147:C:H2'	1:A:1148:U:H6	1.82	0.43
11:K:48:ILE:O	11:K:48:ILE:HG12	2.19	0.43
1:A:513:C:H2'	1:A:514:C:C6	2.53	0.43
14:N:44:LEU:HD12	14:N:48:ALA:HB2	2.00	0.43
6:F:91:VAL:HG21	18:R:72:ARG:HH12	1.84	0.43
1:A:1355:G:H2'	1:A:1356:G:C8	2.53	0.43
3:C:52:LEU:HG	3:C:52:LEU:O	2.18	0.43
1:A:996:A:H2	1:A:1045:C:H2'	1.84	0.43
1:A:1279:A:H61	3:C:26:LYS:NZ	2.16	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1127:G:H1'	1:A:1148:U:N3	2.34	0.43
1:A:1076:C:N4	1:A:1081:G:H1	2.15	0.43
1:A:769:G:H4'	1:A:1513:A:H4'	2.01	0.43
1:A:1089:G:C5	1:A:1090:U:C4	3.06	0.43
1:A:203:U:H3'	1:A:203:U:P	2.59	0.43
1:A:922:G:H1'	5:E:19:MET:HB2	2.00	0.43
2:B:233:SER:OG	2:B:234:PRO:HD2	2.18	0.43
15:O:39:LEU:HD13	15:O:56:LEU:HB2	2.01	0.43
1:A:254:G:OP1	17:Q:67:LYS:O	2.36	0.43
4:D:112:VAL:HG13	4:D:161:ASN:ND2	2.33	0.43
1:A:830:G:H2'	1:A:831:U:O4'	2.19	0.43
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.52	0.43
1:A:1316:G:N2	1:A:1319:A:O5'	2.52	0.43
1:A:1442:G:N7	1:A:1442(A):G:C5	2.87	0.43
1:A:60:A:P	1:A:60:A:H8	2.41	0.43
1:A:663:A:O3'	18:R:64:ARG:NH2	2.41	0.43
13:M:56:LEU:O	13:M:59:TYR:HB3	2.18	0.43
1:A:919:A:O5'	1:A:919:A:H8	2.02	0.43
12:L:70:ILE:HG23	12:L:100:ILE:HD12	2.00	0.43
1:A:929:G:C6	1:A:930:C:C4	3.06	0.43
1:A:380:G:C2	1:A:384:G:C6	3.06	0.43
3:C:111:LEU:HA	3:C:202:ILE:HG21	1.99	0.43
2:B:118:LEU:HA	2:B:121:LEU:HB3	2.00	0.43
1:A:1247:U:H1'	1:A:1291:G:H22	1.84	0.43
1:A:953:G:H2'	1:A:954:G:O4'	2.18	0.43
1:A:826:C:H2'	1:A:827:U:H6	1.84	0.43
3:C:20:SER:HB2	3:C:22:TRP:NE1	2.33	0.43
5:E:55:VAL:O	5:E:58:ALA:HB3	2.19	0.43
1:A:91:C:H2'	1:A:92:C:C6	2.54	0.43
2:B:216:SER:O	2:B:220:ASP:N	2.40	0.43
1:A:1130:A:H1'	1:A:1146:A:C2	2.53	0.43
1:A:1135:U:H4'	1:A:1136:U:C4	2.53	0.43
1:A:538:G:OP1	12:L:114:LYS:N	2.44	0.43
1:A:542:G:H2'	1:A:543:C:C6	2.53	0.43
1:A:954:G:C2	1:A:955:U:C2	3.07	0.43
1:A:445:G:C6	1:A:490:G:C6	3.07	0.43
1:A:1090:U:O5'	1:A:1090:U:H6	2.01	0.43
7:G:101:LEU:O	7:G:105:VAL:HG23	2.18	0.43
1:A:1207:G:H2'	1:A:1208:C:O4'	2.18	0.43
1:A:325:A:H2'	1:A:326:G:O4'	2.18	0.43
1:A:1493:A:O2'	1:A:1494:G:H8	2.02	0.43
1:A:1239:A:H61	1:A:1296:C:H2'	1.84	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:157:ARG:HG2	2:B:158:LEU:N	2.33	0.43
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.99	0.43
1:A:1036:G:H5''	1:A:1037:C:H5	1.84	0.43
1:A:1291:G:C6	1:A:1292:U:C4	3.07	0.43
1:A:1106:G:H2'	1:A:1107:C:H6	1.84	0.43
1:A:613:C:N4	1:A:627:G:H1	2.16	0.43
1:A:1412:C:H2'	1:A:1413:A:C8	2.53	0.43
2:B:149:LEU:HB3	2:B:152:PHE:CB	2.49	0.43
7:G:32:ARG:O	7:G:35:LYS:HG3	2.19	0.43
3:C:46:GLU:CD	3:C:46:GLU:H	2.21	0.43
5:E:6:PHE:HA	5:E:6:PHE:HD2	1.74	0.43
1:A:586:C:C2'	1:A:587:G:H5'	2.49	0.43
10:J:50:ILE:HG23	10:J:57:LYS:HA	2.00	0.43
20:T:41:ILE:H	20:T:41:ILE:HG13	1.26	0.43
1:A:1266:G:N2	1:A:1268:A:C8	2.85	0.43
1:A:31:G:H5'	1:A:306:G:N2	2.34	0.43
1:A:1259:C:H2'	1:A:1283:G:O2'	2.19	0.43
4:D:205:GLU:OE1	5:E:100:VAL:HB	2.19	0.43
7:G:70:LYS:HA	7:G:71:PRO:HD3	1.76	0.43
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.91	0.43
1:A:1356:G:C6	1:A:1357:A:C6	3.07	0.42
1:A:227:G:H2'	1:A:228:A:C8	2.54	0.42
18:R:52:PRO:O	18:R:56:THR:HG23	2.19	0.42
8:H:118:VAL:C	8:H:119:LEU:HD23	2.39	0.42
2:B:84:GLU:HA	2:B:87:ARG:HB3	2.00	0.42
1:A:602:A:C6	1:A:637:G:C6	3.07	0.42
12:L:85:ILE:HD13	12:L:85:ILE:HA	1.70	0.42
1:A:1442:G:H2'	1:A:1442(A):G:C8	2.54	0.42
1:A:960:U:H4'	1:A:961:U:C5'	2.49	0.42
1:A:1089:G:C6	1:A:1090:U:N3	2.87	0.42
1:A:512:U:H2'	1:A:513:C:H6	1.83	0.42
1:A:658:G:C5	1:A:659:U:C5	3.07	0.42
1:A:375:U:H2'	1:A:376:G:C8	2.54	0.42
3:C:137:ALA:O	3:C:140:ARG:HB2	2.19	0.42
1:A:1140:C:H2'	1:A:1141:C:H6	1.84	0.42
3:C:114:PRO:CA	3:C:185:GLY:HA3	2.49	0.42
1:A:1128:C:H5'	9:I:16:ARG:HH12	1.84	0.42
2:B:42:ILE:HG21	2:B:202:PRO:O	2.19	0.42
8:H:39:LEU:H	8:H:39:LEU:HD22	1.85	0.42
1:A:1268:A:N6	1:A:1269:A:N6	2.67	0.42
2:B:20:GLU:O	2:B:40:HIS:HB2	2.20	0.42
1:A:1022:G:H2'	1:A:1023:G:H8	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1226:C:H4'	19:S:80:TYR:OH	2.19	0.42
1:A:522:C:H5''	12:L:120:TYR:HH	1.79	0.42
1:A:1174:G:H2'	1:A:1175:G:H8	1.84	0.42
1:A:1084:G:C5	1:A:1085:U:C5	3.07	0.42
1:A:99:U:H2'	1:A:100:C:C6	2.54	0.42
1:A:1457:G:N2	1:A:1458:G:H1'	2.34	0.42
1:A:1458:G:H5'	20:T:31:SER:CB	2.50	0.42
1:A:1067:A:N3	1:A:1068:G:H1'	2.34	0.42
2:B:27:LYS:CB	2:B:194:PRO:HD2	2.49	0.42
12:L:45:PRO:HG3	12:L:53:ARG:HH11	1.82	0.42
11:K:32:ILE:HD11	11:K:68:ALA:HB1	2.00	0.42
1:A:453:A:C5	1:A:454:C:C4	3.07	0.42
2:B:163:PHE:HD1	2:B:164:VAL:N	2.17	0.42
1:A:664:G:H22	1:A:741:G:H1	1.68	0.42
1:A:431:A:H2'	1:A:432:A:O4'	2.19	0.42
3:C:43:LEU:HD23	3:C:43:LEU:HA	1.61	0.42
11:K:21:ILE:HA	11:K:30:VAL:HG12	2.01	0.42
1:A:76:C:H3'	1:A:77:G:H5''	2.00	0.42
3:C:23:TYR:CZ	3:C:25:GLY:HA3	2.55	0.42
4:D:200:GLU:OE2	4:D:200:GLU:N	2.52	0.42
15:O:75:PRO:O	15:O:77:ARG:N	2.52	0.42
1:A:1435:G:H2'	1:A:1436:U:C6	2.55	0.42
1:A:909:A:H2'	1:A:910:C:O4'	2.20	0.42
1:A:1350:A:H2'	1:A:1351:U:O4'	2.19	0.42
1:A:1443:G:H1	1:A:1459:C:C2'	2.31	0.42
1:A:960:U:H4'	1:A:961:U:H5''	2.01	0.42
1:A:520:A:O2'	12:L:73:GLU:HG2	2.19	0.42
1:A:1329:A:C2	1:A:1330:U:H1'	2.54	0.42
16:P:17:TYR:N	16:P:17:TYR:HD1	2.18	0.42
14:N:48:ALA:HB2	14:N:53:LEU:HD12	2.00	0.42
1:A:1311:G:C2	1:A:1327:C:C2	3.08	0.42
1:A:730:G:C5	1:A:731:G:H1'	2.54	0.42
8:H:25:ASP:HB3	8:H:58:TYR:HD2	1.85	0.42
17:Q:58:GLU:OE1	17:Q:75:ARG:NH1	2.53	0.42
2:B:167:PRO:O	2:B:174:VAL:HG21	2.19	0.42
1:A:961:U:H2'	1:A:962:C:O4'	2.19	0.42
1:A:965:A:H5'	1:A:969:A:H5''	2.01	0.42
1:A:432:A:H3'	1:A:433:C:C6	2.55	0.42
1:A:1307:U:H5''	13:M:101:GLN:NE2	2.34	0.42
2:B:98:LEU:O	2:B:101:MET:HB2	2.20	0.42
1:A:1300:G:O2'	1:A:1301:U:P	2.77	0.42
1:A:1297:C:O3'	7:G:114:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:121:VAL:O	4:D:134:ASP:HA	2.20	0.42
1:A:113:G:H2'	1:A:114:U:C6	2.54	0.42
15:O:74:ASP:OD2	15:O:77:ARG:HB2	2.19	0.42
1:A:701:C:OP1	1:A:702:A:O2'	2.31	0.42
1:A:1030(B):C:H3'	1:A:1030(C):G:C8	2.54	0.42
8:H:11:THR:HA	8:H:14:ARG:NH1	2.35	0.42
1:A:1385:G:C6	1:A:1386:G:N7	2.87	0.42
13:M:68:GLY:HA2	13:M:71:ARG:HB2	2.01	0.42
3:C:150:LYS:O	3:C:201:TYR:HB2	2.20	0.42
1:A:60:A:H8	1:A:60:A:OP1	2.02	0.42
1:A:1111:A:N6	3:C:177:THR:HA	2.35	0.42
1:A:624:C:H4'	16:P:10:GLY:HA2	2.01	0.42
1:A:864:A:H2'	1:A:865:A:C8	2.55	0.42
14:N:47:LEU:HD23	14:N:50:LYS:HD2	2.01	0.42
1:A:867:G:H5'	22:V:3:ARG:CB	2.49	0.42
10:J:46:ARG:HD3	14:N:61:TRP:CZ3	2.55	0.42
2:B:69:LEU:HB2	2:B:162:ILE:HG22	2.02	0.42
10:J:32:ALA:HB1	10:J:33:GLN:HB3	2.02	0.42
1:A:72:C:C2	1:A:98:G:N2	2.88	0.42
5:E:60:TYR:C	5:E:60:TYR:CD1	2.93	0.42
16:P:28:ARG:HH11	16:P:28:ARG:CG	2.26	0.42
1:A:539:A:OP2	12:L:115:LYS:NZ	2.53	0.42
1:A:1441:G:O2'	1:A:1459:C:C4	2.64	0.42
1:A:1106:G:H2'	1:A:1107:C:C6	2.55	0.42
4:D:79:PHE:CD2	4:D:80:GLU:N	2.82	0.42
1:A:742:G:OP1	15:O:59:MET:HE2	2.19	0.42
5:E:78:HIS:CE1	5:E:142:LEU:HA	2.50	0.42
1:A:1363(A):A:H4'	1:A:1364:U:O5'	2.20	0.42
1:A:626:U:H4'	16:P:38:TYR:CZ	2.54	0.42
1:A:437:U:H2'	1:A:438:G:C8	2.55	0.42
1:A:185:A:C6	1:A:186:C:C4	3.08	0.42
1:A:1064:G:H8	1:A:1064:G:O5'	2.02	0.42
1:A:375:U:P	16:P:69:THR:HG21	2.60	0.42
1:A:967:C:O5'	1:A:967:C:H6	2.02	0.42
12:L:84:LEU:HD22	12:L:85:ILE:H	1.85	0.42
1:A:606:G:H5''	1:A:607:A:H5'	2.02	0.42
13:M:9:ILE:N	13:M:10:PRO:HD3	2.35	0.42
1:A:1525:G:OP1	11:K:120:ARG:NH2	2.52	0.42
1:A:1165:C:H2'	1:A:1166:G:H8	1.84	0.42
1:A:118:U:C5	1:A:288:A:C6	3.08	0.42
1:A:1033:G:H2'	1:A:1034:G:O4'	2.20	0.41
1:A:160:A:N6	1:A:346:G:N2	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1333:A:C6	1:A:1334:G:C4	3.08	0.41
1:A:1353:G:H5''	21:U:13:ILE:CG2	2.49	0.41
1:A:510:A:H5''	1:A:511:C:OP2	2.19	0.41
1:A:586:C:H2'	1:A:587:G:H5'	2.02	0.41
1:A:597:G:N2	8:H:94:TYR:OH	2.53	0.41
1:A:649:G:H2'	1:A:650:G:C8	2.55	0.41
1:A:924:C:H2'	1:A:925:G:H8	1.84	0.41
8:H:121:ASP:O	8:H:125:ARG:HG2	2.20	0.41
7:G:16:LEU:HD12	9:I:42:ARG:HA	2.02	0.41
19:S:28:LYS:O	19:S:47:HIS:HD2	2.03	0.41
12:L:46:LYS:HG3	12:L:92:ASP:HA	2.01	0.41
7:G:74:GLU:O	7:G:88:PRO:HA	2.20	0.41
1:A:951:G:O6	13:M:105:THR:HG21	2.20	0.41
1:A:1360:A:OP2	14:N:35:ARG:NH2	2.40	0.41
13:M:65:LYS:O	13:M:65:LYS:HE3	2.20	0.41
2:B:42:ILE:HD13	2:B:203:GLY:HA2	2.03	0.41
16:P:17:TYR:CD1	16:P:17:TYR:N	2.87	0.41
1:A:532:A:N6	3:C:193:TYR:HB3	2.35	0.41
1:A:1092:A:C6	1:A:1183:A:C2	3.08	0.41
1:A:477:A:H2'	1:A:479:C:H6	1.84	0.41
15:O:74:ASP:HA	15:O:75:PRO:HD2	1.76	0.41
1:A:1050:G:H2'	1:A:1051:C:C6	2.55	0.41
1:A:146:G:H5''	1:A:147:G:OP2	2.20	0.41
1:A:106:C:H2'	1:A:107:G:H8	1.84	0.41
7:G:113:GLU:HG2	7:G:113:GLU:O	2.20	0.41
1:A:1352:C:H2'	1:A:1353:G:C8	2.54	0.41
1:A:390:C:H2'	1:A:391:G:C8	2.55	0.41
2:B:163:PHE:HA	2:B:185:ILE:O	2.20	0.41
1:A:826:C:H2'	1:A:827:U:C6	2.55	0.41
1:A:1080:A:H5''	1:A:1081:G:OP2	2.21	0.41
1:A:708:C:P	11:K:85:ARG:HH22	2.44	0.41
8:H:119:LEU:HB3	8:H:123:GLU:HB2	2.02	0.41
1:A:777:A:C2	11:K:119:CYS:HB3	2.55	0.41
2:B:16:HIS:CD2	2:B:210:SER:HA	2.55	0.41
1:A:1429:C:H2'	1:A:1430:C:C6	2.54	0.41
19:S:67:VAL:HB	19:S:68:GLY:H	1.68	0.41
2:B:74:LYS:HD3	2:B:205:ASP:O	2.21	0.41
17:Q:27:PHE:HD1	17:Q:28:PRO:O	2.03	0.41
9:I:112:LYS:CG	9:I:119:ALA:HB2	2.51	0.41
1:A:373:A:H61	1:A:391:G:H1'	1.85	0.41
15:O:87:ILE:HG23	15:O:88:ARG:N	2.35	0.41
1:A:1443:G:O6	1:A:1459:C:C2	2.73	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1291:G:O2'	1:A:1292:U:H5'	2.20	0.41
15:O:81:LEU:O	15:O:85:LEU:N	2.51	0.41
10:J:50:ILE:HD11	10:J:60:ARG:NH1	2.35	0.41
1:A:393:A:C2	1:A:394:G:C8	3.08	0.41
12:L:32:PHE:CE1	12:L:86:ARG:HG3	2.52	0.41
14:N:53:LEU:HA	14:N:54:PRO:HD3	1.73	0.41
1:A:721:G:H4'	1:A:722:A:O4'	2.20	0.41
15:O:76:GLU:O	15:O:79:ARG:N	2.53	0.41
12:L:30:ALA:HA	12:L:31:PRO:HD3	1.79	0.41
5:E:39:GLY:O	5:E:69:VAL:HG12	2.20	0.41
1:A:1113:C:H2'	1:A:1114:C:C6	2.54	0.41
1:A:788:U:H2'	1:A:789:U:O4'	2.21	0.41
1:A:1286:A:N6	1:A:1354:C:O3'	2.53	0.41
1:A:1179:A:OP1	1:A:1179:A:C8	2.74	0.41
1:A:1446:U:O2	1:A:1456:G:N2	2.53	0.41
3:C:69:HIS:CD2	3:C:104:GLN:HB2	2.55	0.41
1:A:300:A:H1'	1:A:565:U:O2	2.21	0.41
1:A:271:C:H2'	1:A:272:C:H6	1.85	0.41
1:A:619:U:C2	4:D:135:LEU:HD22	2.56	0.41
17:Q:22:LEU:HD12	17:Q:40:LYS:O	2.20	0.41
12:L:47:LYS:HE2	12:L:47:LYS:HB2	1.83	0.41
9:I:45:ALA:CB	9:I:47:LEU:H	2.33	0.41
1:A:957:U:H4'	19:S:79:THR:OG1	2.20	0.41
14:N:25:VAL:HB	14:N:39:LEU:HD21	2.01	0.41
15:O:3:ILE:HD13	15:O:3:ILE:H	1.84	0.41
1:A:1163:C:H2'	1:A:1164:G:H8	1.85	0.41
1:A:1349:A:H2'	1:A:1350:A:O4'	2.21	0.41
19:S:33:THR:O	19:S:52:TYR:HB2	2.20	0.41
1:A:373:A:H2'	1:A:374:A:H8	1.84	0.41
1:A:1245:A:N1	1:A:1293:G:C6	2.89	0.41
1:A:971:G:H1	1:A:1363(A):A:H5'	1.85	0.41
5:E:37:ARG:HG2	5:E:37:ARG:NH1	2.35	0.41
1:A:980:C:H5'	1:A:981:U:OP2	2.20	0.41
1:A:33:A:H2'	1:A:34:C:C6	2.55	0.41
1:A:263:A:OP1	20:T:79:ARG:NH1	2.54	0.41
1:A:376:G:H5''	16:P:5:ARG:CB	2.51	0.41
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.20	0.41
4:D:188:LEU:HG	4:D:188:LEU:H	1.24	0.41
22:V:45:ARG:O	22:V:49:ALA:HB2	2.21	0.41
3:C:111:LEU:HD11	3:C:144:SER:HB3	2.03	0.41
1:A:509:A:HO2'	1:A:510:A:P	2.40	0.41
2:B:167:PRO:HG2	2:B:192:SER:CB	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:85:ARG:HD3	8:H:86:ILE:N	2.35	0.41
17:Q:91:ARG:O	17:Q:94:ASN:HB2	2.20	0.41
1:A:825:G:H2'	1:A:826:C:C6	2.55	0.41
1:A:34:C:H42	1:A:550:G:H1	1.69	0.41
22:V:30:PRO:HG3	22:V:40:TRP:CZ3	2.56	0.41
11:K:69:ALA:O	11:K:72:ALA:N	2.48	0.41
2:B:133:LYS:O	2:B:137:ARG:N	2.31	0.41
1:A:129(A):G:C6	1:A:189(H):G:H1'	2.55	0.41
1:A:1163:C:C4	1:A:1164:G:N7	2.89	0.41
1:A:1273:G:H3'	1:A:1274:G:C8	2.31	0.41
1:A:374:A:H2'	1:A:374:A:N3	2.36	0.41
1:A:1443:G:O6	1:A:1459:C:O2	2.38	0.41
1:A:1155:G:C6	1:A:1156:G:C6	3.09	0.41
9:I:9:ARG:HB2	9:I:9:ARG:NH1	2.31	0.41
1:A:954:G:C6	13:M:104:ARG:NH1	2.88	0.41
10:J:54:PHE:CG	10:J:55:LYS:N	2.88	0.41
1:A:938:A:N6	1:A:939:G:C6	2.89	0.41
16:P:16:HIS:C	16:P:17:TYR:HD1	2.24	0.41
1:A:15:G:H4'	5:E:24:ARG:NH1	2.34	0.41
1:A:175:C:H2'	1:A:176:C:C6	2.56	0.41
2:B:79:ASP:O	2:B:82:ARG:N	2.54	0.41
4:D:93:PHE:O	4:D:97:LEU:HB2	2.20	0.41
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.56	0.41
1:A:416:G:H2'	1:A:417:C:O4'	2.20	0.41
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.86	0.41
1:A:1047:G:H1'	1:A:1215:G:O2'	2.20	0.41
1:A:976:G:OP1	14:N:31:ARG:HD3	2.21	0.41
1:A:1392:G:N2	1:A:1502:A:H8	2.13	0.41
1:A:1319:A:N1	1:A:1323:G:H1'	2.35	0.41
1:A:521:G:H2'	1:A:522:C:H6	1.86	0.41
1:A:1291:G:C2'	1:A:1292:U:H5'	2.50	0.41
1:A:1107:C:N4	1:A:1108:G:N7	2.69	0.41
1:A:1084:G:C6	1:A:1085:U:C4	3.08	0.41
4:D:174:LEU:HA	4:D:174:LEU:HD23	1.82	0.41
9:I:100:GLY:O	9:I:103:THR:HG22	2.20	0.41
1:A:970:C:H41	9:I:126:SER:CB	2.34	0.41
3:C:16:ARG:HD2	3:C:54:ARG:NH2	2.36	0.41
8:H:73:ASP:OD2	8:H:75:ARG:HD3	2.21	0.41
19:S:69:HIS:HD2	19:S:74:PHE:HE1	1.69	0.41
13:M:3:ARG:HE	13:M:4:ILE:HG22	1.86	0.41
3:C:6:HIS:HE1	3:C:184:TYR:CD2	2.39	0.41
8:H:38:ILE:HD12	8:H:118:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:116:ALA:HA	7:G:119:ARG:HB2	2.03	0.41
9:I:12:GLU:O	9:I:67:GLY:HA3	2.20	0.41
1:A:111:G:O6	1:A:330:C:N4	2.52	0.41
1:A:1182:G:H4'	1:A:1183:A:H5'	2.02	0.41
2:B:22:LYS:H	2:B:40:HIS:HD2	1.68	0.41
5:E:66:MET:O	5:E:67:VAL:HB	2.20	0.41
1:A:1253:G:H2'	1:A:1254:C:C6	2.56	0.41
8:H:44:PHE:HA	8:H:79:VAL:CG1	2.51	0.41
2:B:194:PRO:C	2:B:196:LEU:H	2.24	0.41
13:M:20:THR:HG23	13:M:26:GLY:HA2	2.03	0.41
1:A:189(C):C:H2'	1:A:189(D):C:O4'	2.20	0.41
1:A:641:U:O3'	1:A:642:A:H8	2.03	0.41
6:F:76:ALA:O	6:F:80:ARG:HG3	2.21	0.41
1:A:1109:C:H2'	1:A:1110:A:O4'	2.21	0.41
18:R:85:LEU:HD22	18:R:86:VAL:N	2.35	0.41
1:A:986:A:H2'	1:A:987:G:O4'	2.20	0.41
1:A:342:C:C2	1:A:348:G:N2	2.89	0.41
3:C:132:ARG:O	3:C:136:GLN:HB2	2.20	0.41
11:K:99:GLN:HA	11:K:105:VAL:HG11	2.03	0.41
1:A:1465:C:H2'	1:A:1466:C:O4'	2.21	0.41
11:K:20:TYR:CE2	11:K:83:ILE:HD12	2.55	0.41
15:O:18:PHE:HD1	15:O:20:GLY:H	1.69	0.41
2:B:116:GLU:HA	2:B:119:GLU:HB2	2.03	0.41
1:A:1236:A:O2'	1:A:1304:G:H4'	2.21	0.41
1:A:373:A:C8	1:A:482:A:C8	3.09	0.41
1:A:391:G:C6	1:A:392:G:C5	3.09	0.41
1:A:509:A:O2'	1:A:510:A:OP1	2.29	0.41
1:A:1072:G:O2'	1:A:1073:U:H5'	2.20	0.41
1:A:1203:C:H2'	1:A:1204:A:O4'	2.20	0.41
1:A:828:A:H5''	1:A:859:A:C2	2.56	0.41
1:A:707:C:OP1	11:K:85:ARG:NH1	2.54	0.41
1:A:925:G:C2	1:A:927:G:C8	3.09	0.41
13:M:63:THR:HG23	13:M:64:TRP:CD1	2.56	0.41
3:C:130:VAL:O	3:C:134:ILE:HG13	2.21	0.41
2:B:224:GLN:HB2	2:B:229:VAL:HG22	2.02	0.41
1:A:57:G:H2'	1:A:58:C:O4'	2.21	0.41
1:A:107:G:H2'	1:A:108:G:O4'	2.21	0.41
15:O:76:GLU:O	15:O:80:ALA:N	2.53	0.41
4:D:6:GLY:O	4:D:8:VAL:N	2.53	0.41
1:A:994:A:H61	1:A:1047:G:C4'	2.34	0.40
1:A:1288:A:H61	1:A:1371:G:HO2'	1.68	0.40
1:A:390:C:H2'	1:A:391:G:H8	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:689:C:P	11:K:46:GLY:HA3	2.61	0.40
3:C:47:LEU:HD23	3:C:47:LEU:HA	1.89	0.40
1:A:246:A:N3	1:A:247:G:H1'	2.36	0.40
1:A:175:C:H2'	1:A:176:C:H6	1.85	0.40
1:A:731:G:OP1	1:A:766:A:H1'	2.20	0.40
1:A:865:A:O5'	1:A:865:A:H8	2.04	0.40
1:A:1168:A:C6	1:A:1169:A:C6	3.09	0.40
1:A:790:A:N1	1:A:1497:G:H5''	2.36	0.40
11:K:31:THR:HG22	11:K:42:TRP:CB	2.51	0.40
6:F:91:VAL:HG11	18:R:72:ARG:NH1	2.32	0.40
1:A:1370:G:O2'	1:A:1371:G:H5'	2.21	0.40
1:A:940:C:HO2'	1:A:1374:A:H2	1.69	0.40
1:A:1274:G:H21	1:A:1275:A:N6	2.14	0.40
1:A:1015:A:C2	1:A:1218:C:O2	2.72	0.40
1:A:673:G:H5''	6:F:87:ARG:CZ	2.51	0.40
13:M:96:LEU:HA	13:M:97:PRO:HD3	1.88	0.40
1:A:1511:G:H2'	1:A:1512:U:O4'	2.21	0.40
1:A:622:A:C8	1:A:623:C:C5	3.09	0.40
1:A:1151:A:O4'	10:J:39:PRO:HB2	2.20	0.40
5:E:107:ARG:O	5:E:111:GLU:N	2.53	0.40
1:A:189:G:H2'	1:A:189(A):C:C6	2.56	0.40
3:C:57:ILE:HG12	3:C:66:VAL:HA	2.03	0.40
2:B:55:PHE:HD2	2:B:55:PHE:HA	1.77	0.40
1:A:1039:C:H2'	1:A:1040:U:O4'	2.21	0.40
1:A:1342:C:H2'	1:A:1343:G:C8	2.57	0.40
1:A:1152:A:H5'	10:J:13:HIS:CD2	2.57	0.40
1:A:1073:U:O2'	2:B:104:ASN:OD1	2.23	0.40
1:A:1264:C:H2'	1:A:1265:G:H8	1.82	0.40
1:A:881:G:OP2	12:L:12:ARG:NH2	2.54	0.40
1:A:658:G:H2'	1:A:659:U:C6	2.56	0.40
1:A:981:U:H4'	14:N:21:TYR:CZ	2.56	0.40
13:M:33:ALA:HB2	13:M:64:TRP:CZ3	2.56	0.40
1:A:1269:A:C4	1:A:1313:U:H1'	2.56	0.40
20:T:74:LYS:HB3	20:T:74:LYS:HE2	1.88	0.40
15:O:36:ILE:O	15:O:39:LEU:N	2.55	0.40
1:A:791:G:O5'	1:A:791:G:H8	2.04	0.40
4:D:6:GLY:O	4:D:8:VAL:HG23	2.21	0.40
5:E:149:GLU:HG2	5:E:149:GLU:H	1.53	0.40
2:B:118:LEU:O	2:B:122:PHE:N	2.55	0.40
1:A:519:C:H2'	1:A:520:A:H8	1.85	0.40
1:A:1057:G:C5	1:A:1204:A:C2	3.10	0.40
1:A:1079:G:C6	1:A:1080:A:N6	2.90	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:30:PRO:HB2	22:V:31:TYR:HB2	2.04	0.40
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.21	0.40
1:A:786:G:C2	1:A:797:C:C2	3.09	0.40
1:A:9:G:OP1	5:E:122:GLU:HB2	2.22	0.40
1:A:1380:U:C4	7:G:3:ARG:HG2	2.56	0.40
1:A:509:A:C6	1:A:510:A:N1	2.89	0.40
1:A:1107:C:H5''	3:C:173:VAL:N	2.29	0.40
1:A:597:G:H5''	1:A:598:U:OP2	2.21	0.40
1:A:1307:U:O5'	1:A:1307:U:H6	2.04	0.40
1:A:1512:U:H2'	1:A:1513:A:H8	1.86	0.40
1:A:474:G:C2	1:A:475:G:C5	3.09	0.40
1:A:924:C:H2'	1:A:925:G:C8	2.56	0.40
1:A:698:G:C6	1:A:699:C:C4	3.10	0.40
1:A:1403:C:O5'	1:A:1403:C:H6	2.04	0.40
22:V:13:HIS:ND1	22:V:13:HIS:O	2.46	0.40
11:K:29:ILE:HG12	11:K:44:SER:HB2	2.03	0.40
1:A:1109:C:O2'	1:A:1110:A:H5'	2.22	0.40
11:K:17:GLY:HA2	11:K:35:PRO:HD3	2.03	0.40
1:A:217:C:O2'	1:A:470:C:N4	2.55	0.40
18:R:34:TYR:CD2	18:R:34:TYR:N	2.89	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%)	192 (85%)	33 (14%)	2 (1%)	25	73
3	C	204/239 (85%)	177 (87%)	27 (13%)	0	100	100
4	D	206/209 (99%)	180 (87%)	24 (12%)	2 (1%)	22	70
5	E	146/162 (90%)	126 (86%)	20 (14%)	0	100	100
6	F	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
7	G	153/156 (98%)	128 (84%)	23 (15%)	2 (1%)	18	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
9	I	123/128 (96%)	109 (89%)	12 (10%)	2 (2%)	14	56
10	J	94/105 (90%)	74 (79%)	18 (19%)	2 (2%)	11	47
11	K	112/129 (87%)	100 (89%)	12 (11%)	0	100	100
12	L	120/132 (91%)	107 (89%)	11 (9%)	2 (2%)	14	54
13	M	112/126 (89%)	84 (75%)	27 (24%)	1 (1%)	25	73
14	N	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	14	54
15	O	86/89 (97%)	72 (84%)	14 (16%)	0	100	100
16	P	80/88 (91%)	71 (89%)	7 (9%)	2 (2%)	9	40
17	Q	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
18	R	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
19	S	79/93 (85%)	60 (76%)	16 (20%)	3 (4%)	5	27
20	T	95/106 (90%)	81 (85%)	11 (12%)	3 (3%)	6	33
21	U	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
22	V	51/61 (84%)	34 (67%)	14 (28%)	3 (6%)	2	14
All	All	2364/2599 (91%)	2024 (86%)	315 (13%)	25 (1%)	21	67

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	92	ASP
2	B	129	GLU
16	P	53	VAL
19	S	47	HIS
20	T	100	ILE
22	V	27	GLU
10	J	56	HIS
13	M	5	ALA
2	B	9	GLU
16	P	79	VAL
20	T	10	LEU
22	V	30	PRO
9	I	23	ASN
9	I	56	LEU
10	J	57	LYS
12	L	28	LYS
14	N	59	ALA

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Mol	Chain	Res	Type
19	S	12	ASP
19	S	67	VAL
4	D	7	PRO
7	G	112	PRO
4	D	178	VAL
22	V	53	VAL
7	G	55	GLY
20	T	98	PRO

### 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%)	135 (76%)	42 (24%)	1	5
3	C	114/188 (61%)	78 (68%)	36 (32%)	0	2
4	D	141/181 (78%)	114 (81%)	27 (19%)	2	12
5	E	108/123 (88%)	84 (78%)	24 (22%)	1	7
6	F	76/90 (84%)	69 (91%)	7 (9%)	13	46
7	G	103/127 (81%)	77 (75%)	26 (25%)	1	4
8	H	103/119 (87%)	84 (82%)	19 (18%)	2	13
9	I	62/99 (63%)	48 (77%)	14 (23%)	1	6
10	J	53/92 (58%)	39 (74%)	14 (26%)	1	4
11	K	81/99 (82%)	70 (86%)	11 (14%)	5	24
12	L	91/109 (84%)	79 (87%)	12 (13%)	6	25
13	M	64/101 (63%)	49 (77%)	15 (23%)	1	5
14	N	46/50 (92%)	33 (72%)	13 (28%)	0	3
15	O	77/80 (96%)	71 (92%)	6 (8%)	18	55
16	P	63/74 (85%)	47 (75%)	16 (25%)	1	4
17	Q	94/97 (97%)	80 (85%)	14 (15%)	4	20
18	R	49/77 (64%)	42 (86%)	7 (14%)	5	22
19	S	43/80 (54%)	32 (74%)	11 (26%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	65/82 (79%)	55 (85%)	10 (15%)	4	19
21	U	18/22 (82%)	13 (72%)	5 (28%)	0	3
22	V	21/50 (42%)	14 (67%)	7 (33%)	0	2
All	All	1649/2160 (76%)	1313 (80%)	336 (20%)	2	9

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	17	PHE
2	B	21	ARG
2	B	32	ILE
2	B	37	ASN
2	B	45	GLN
2	B	47	THR
2	B	49	GLU
2	B	51	LEU
2	B	58	ILE
2	B	67	THR
2	B	69	LEU
2	B	75	LYS
2	B	80	ILE
2	B	87	ARG
2	B	93	VAL
2	B	94	ASN
2	B	114	ARG
2	B	119	GLU
2	B	122	PHE
2	B	130	ARG
2	B	139	LYS
2	B	140	HIS
2	B	145	LEU
2	B	149	LEU
2	B	157	ARG
2	B	158	LEU
2	B	163	PHE
2	B	169	LYS
2	B	170	GLU
2	B	172	ILE
2	B	187	LEU
2	B	189	ASP

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Mol	Chain	Res	Type
2	B	191	ASP
2	B	200	ILE
2	B	206	ASP
2	B	214	ILE
2	B	215	LEU
2	B	224	GLN
2	B	226	ARG
2	B	231	GLU
2	B	233	SER
3	C	5	ILE
3	C	6	HIS
3	C	8	ILE
3	C	12	LEU
3	C	18	TRP
3	C	30	ARG
3	C	31	HIS
3	C	32	LEU
3	C	33	LEU
3	C	34	LEU
3	C	36	ASP
3	C	37	GLN
3	C	46	GLU
3	C	48	TYR
3	C	49	SER
3	C	52	LEU
3	C	55	VAL
3	C	58	GLU
3	C	59	ARG
3	C	102	ASN
3	C	111	LEU
3	C	118	GLN
3	C	131	ARG
3	C	136	GLN
3	C	150	LYS
3	C	152	ILE
3	C	170	GLN
3	C	172	ARG
3	C	173	VAL
3	C	175	LEU
3	C	178	LEU
3	C	179	ARG
3	C	182	ILE

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Mol	Chain	Res	Type
3	C	188	LEU
3	C	192	THR
3	C	193	TYR
4	D	11	LEU
4	D	22	LYS
4	D	34	GLU
4	D	36	ARG
4	D	57	ARG
4	D	58	LEU
4	D	73	ARG
4	D	77	ASN
4	D	79	PHE
4	D	83	SER
4	D	97	LEU
4	D	104	VAL
4	D	106	TYR
4	D	107	ARG
4	D	110	PHE
4	D	126	ILE
4	D	127	THR
4	D	135	LEU
4	D	137	SER
4	D	138	TYR
4	D	158	ILE
4	D	160	GLN
4	D	181	MET
4	D	188	LEU
4	D	193	ASP
4	D	196	LEU
4	D	200	GLU
5	E	5	ASP
5	E	6	PHE
5	E	12	LEU
5	E	16	THR
5	E	20	GLN
5	E	34	VAL
5	E	37	ARG
5	E	41	VAL
5	E	47	LYS
5	E	53	LEU
5	E	60	TYR
5	E	75	THR

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Mol	Chain	Res	Type
5	E	76	ILE
5	E	78	HIS
5	E	79	GLU
5	E	82	VAL
5	E	89	ILE
5	E	91	LEU
5	E	117	ASP
5	E	121	LYS
5	E	137	GLU
5	E	144	THR
5	E	147	ASP
5	E	149	GLU
6	F	22	GLU
6	F	36	ARG
6	F	43	LEU
6	F	55	ASP
6	F	69	GLU
6	F	82	ARG
6	F	83	ASP
7	G	6	ARG
7	G	10	ARG
7	G	12	LEU
7	G	24	THR
7	G	30	ILE
7	G	32	ARG
7	G	33	ASP
7	G	38	LEU
7	G	51	GLN
7	G	53	LYS
7	G	59	LEU
7	G	72	ARG
7	G	74	GLU
7	G	75	VAL
7	G	94	ARG
7	G	104	LEU
7	G	113	GLU
7	G	114	ARG
7	G	122	HIS
7	G	142	GLU
7	G	143	ARG
7	G	144	MET
7	G	146	GLU

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Mol	Chain	Res	Type
7	G	151	TYR
7	G	153	HIS
7	G	155	ARG
8	H	3	THR
8	H	8	ASP
8	H	19	VAL
8	H	21	LYS
8	H	24	THR
8	H	25	ASP
8	H	42	GLU
8	H	45	ILE
8	H	49	GLU
8	H	78	GLN
8	H	84	ARG
8	H	85	ARG
8	H	91	ARG
8	H	95	VAL
8	H	109	ILE
8	H	112	LEU
8	H	114	THR
8	H	125	ARG
8	H	137	VAL
9	I	3	GLN
9	I	9	ARG
9	I	29	ASN
9	I	34	ASN
9	I	38	GLN
9	I	41	VAL
9	I	48	GLU
9	I	60	ASP
9	I	64	THR
9	I	87	GLN
9	I	99	LEU
9	I	104	ARG
9	I	107	ARG
9	I	117	HIS
10	J	8	LEU
10	J	9	ARG
10	J	11	PHE
10	J	13	HIS
10	J	16	LEU
10	J	34	VAL

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Mol	Chain	Res	Type
10	J	38	ILE
10	J	43	ARG
10	J	45	ARG
10	J	55	LYS
10	J	58	ASP
10	J	66	ARG
10	J	69	ASN
10	J	96	ILE
11	K	14	VAL
11	K	38	ASN
11	K	48	ILE
11	K	93	GLN
11	K	95	ILE
11	K	96	ARG
11	K	107	SER
11	K	109	VAL
11	K	116	HIS
11	K	119	CYS
11	K	126	ARG
12	L	6	THR
12	L	33	ARG
12	L	43	VAL
12	L	44	THR
12	L	53	ARG
12	L	67	THR
12	L	70	ILE
12	L	92	ASP
12	L	102	ARG
12	L	104	VAL
12	L	118	SER
12	L	123	LYS
13	M	3	ARG
13	M	15	VAL
13	M	16	ASP
13	M	27	LYS
13	M	41	PRO
13	M	47	ASP
13	M	54	VAL
13	M	63	THR
13	M	65	LYS
13	M	70	LEU
13	M	86	CYS

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Mol	Chain	Res	Type
13	M	88	ARG
13	M	98	VAL
13	M	109	THR
13	M	110	ARG
14	N	7	ILE
14	N	8	GLU
14	N	17	LYS
14	N	22	THR
14	N	23	ARG
14	N	24	CYS
14	N	26	ARG
14	N	27	CYS
14	N	29	ARG
14	N	33	VAL
14	N	37	PHE
14	N	41	ARG
14	N	44	LEU
15	O	3	ILE
15	O	35	ARG
15	O	39	LEU
15	O	41	GLU
15	O	62	GLN
15	O	87	ILE
16	P	1	MET
16	P	2	VAL
16	P	3	LYS
16	P	6	LEU
16	P	8	ARG
16	P	28	ARG
16	P	43	LYS
16	P	45	THR
16	P	47	ASP
16	P	52	ASP
16	P	54	GLU
16	P	62	VAL
16	P	67	THR
16	P	69	THR
16	P	71	ARG
16	P	76	GLN
17	Q	9	VAL
17	Q	11	VAL
17	Q	34	LYS

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Mol	Chain	Res	Type
17	Q	45	HIS
17	Q	48	GLU
17	Q	52	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	63	ARG
17	Q	68	ARG
17	Q	72	ARG
17	Q	82	MET
17	Q	93	GLN
17	Q	97	SER
18	R	31	LEU
18	R	32	ARG
18	R	36	ASN
18	R	37	VAL
18	R	53	ARG
18	R	76	LEU
18	R	83	GLU
19	S	7	LYS
19	S	31	ILE
19	S	36	ARG
19	S	37	ARG
19	S	38	SER
19	S	44	MET
19	S	62	ILE
19	S	63	THR
19	S	67	VAL
19	S	77	THR
19	S	81	ARG
20	T	10	LEU
20	T	13	LEU
20	T	22	ARG
20	T	24	LEU
20	T	30	LYS
20	T	41	ILE
20	T	50	GLU
20	T	70	SER
20	T	72	LEU
20	T	93	GLU
21	U	9	ARG
21	U	10	ARG
21	U	12	LYS

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Mol	Chain	Res	Type
21	U	15	ARG
21	U	24	ARG
22	V	4	GLN
22	V	13	HIS
22	V	18	GLN
22	V	31	TYR
22	V	36	GLN
22	V	39	GLN
22	V	48	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	HIS
3	C	104	GLN
3	C	118	GLN
4	D	123	HIS
4	D	129	ASN
4	D	160	GLN
4	D	161	ASN
5	E	78	HIS
7	G	37	ASN
7	G	64	GLN
8	H	78	GLN
9	I	38	GLN
9	I	73	GLN
9	I	87	GLN
9	I	117	HIS
10	J	33	GLN
11	K	93	GLN
12	L	49	ASN
14	N	52	GLN
15	O	37	ASN
16	P	76	GLN
19	S	47	HIS
19	S	69	HIS
19	S	83	HIS
20	T	42	GLN
22	V	4	GLN
22	V	18	GLN
22	V	36	GLN

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1499/1522 (98%)	383 (25%)	29 (1%)

All (383) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	9	G
1	A	10	A
1	A	22	G
1	A	26	A
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	60	A
1	A	61	G
1	A	67	C
1	A	77	G
1	A	78	G
1	A	79	G
1	A	96	U
1	A	97	G
1	A	98	G
1	A	100	C
1	A	101	A
1	A	115	G
1	A	116	A
1	A	119	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	131	C
1	A	144	G
1	A	146	G
1	A	150	C
1	A	160	A
1	A	163	C
1	A	173	U

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Mol	Chain	Res	Type
1	A	182	U
1	A	195	A
1	A	203	U
1	A	204	U
1	A	216	G
1	A	222	U
1	A	231	G
1	A	244	U
1	A	245	C
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	280	C
1	A	281	G
1	A	289	G
1	A	301	G
1	A	306	G
1	A	313	A
1	A	316	G
1	A	321	A
1	A	327	A
1	A	328	C
1	A	332	G
1	A	345	C
1	A	346	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	382	A
1	A	384	G
1	A	388	G
1	A	397	A
1	A	398	C
1	A	409	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	418	C

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Mol	Chain	Res	Type
1	A	421	U
1	A	422	C
1	A	428	G
1	A	429	U
1	A	433	C
1	A	435	C
1	A	436	C
1	A	437	U
1	A	439	A
1	A	442	C
1	A	452	A
1	A	458	C
1	A	461	A
1	A	471	G
1	A	484	G
1	A	485	G
1	A	496	A
1	A	498	U
1	A	500	G
1	A	505	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	521	G
1	A	524	G
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	550	G
1	A	558	G
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	568	G

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Mol	Chain	Res	Type
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	588	G
1	A	592	G
1	A	595	G
1	A	596	C
1	A	597	G
1	A	613	C
1	A	629	G
1	A	630	G
1	A	631	G
1	A	632	A
1	A	650	G
1	A	653	A
1	A	662	G
1	A	665	A
1	A	666	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	752	G
1	A	753	A
1	A	755	G
1	A	777	A
1	A	786	G
1	A	793	U
1	A	794	A
1	A	796	C
1	A	806	C
1	A	816	A
1	A	817	C
1	A	818	G
1	A	821	G
1	A	827	U
1	A	828	A
1	A	829	G
1	A	833	U

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Mol	Chain	Res	Type
1	A	836	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	855	G
1	A	859	A
1	A	864	A
1	A	889	A
1	A	902	G
1	A	913	A
1	A	914	A
1	A	916	G
1	A	925	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	940	C
1	A	960	U
1	A	961	U
1	A	965	A
1	A	966	G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	980	C
1	A	982	U
1	A	983	A
1	A	984	C
1	A	989	C
1	A	992	U
1	A	993	G
1	A	1001	A
1	A	1001(A)	G
1	A	1003	G

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Mol	Chain	Res	Type
1	A	1004	A
1	A	1005	A
1	A	1008	C
1	A	1009	G
1	A	1011	G
1	A	1015	A
1	A	1020	U
1	A	1021	G
1	A	1022	G
1	A	1023	G
1	A	1024	G
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1029	C
1	A	1030(A)	G
1	A	1031	G
1	A	1034	G
1	A	1035	A
1	A	1036	G
1	A	1040	U
1	A	1042	G
1	A	1050	G
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1070	U
1	A	1081	G
1	A	1082	G
1	A	1085	U
1	A	1087	G
1	A	1088	G
1	A	1094	G
1	A	1095	U
1	A	1100	C
1	A	1101	A
1	A	1106	G
1	A	1107	C
1	A	1108	G
1	A	1113	C
1	A	1114	C

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Mol	Chain	Res	Type
1	A	1118	C
1	A	1124	G
1	A	1125	U
1	A	1131	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1147	C
1	A	1152	A
1	A	1154	G
1	A	1157	A
1	A	1159	U
1	A	1171	G
1	A	1172	C
1	A	1174	G
1	A	1178	G
1	A	1181	G
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1185	G
1	A	1193	G
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1202	G
1	A	1206	G
1	A	1208	C
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1220	G
1	A	1225	A
1	A	1227	A
1	A	1228	C
1	A	1229	A
1	A	1238	A
1	A	1239	A
1	A	1241	G

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Mol	Chain	Res	Type
1	A	1244	C
1	A	1250	A
1	A	1252	A
1	A	1254	C
1	A	1255	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1259	C
1	A	1260	C
1	A	1270	C
1	A	1274	G
1	A	1275	A
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1284	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1291	G
1	A	1292	U
1	A	1293	G
1	A	1294	G
1	A	1295	G
1	A	1297	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1306	A
1	A	1309	G
1	A	1310	G
1	A	1312	G
1	A	1316	G
1	A	1319	A
1	A	1320	C
1	A	1321	C

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Mol	Chain	Res	Type
1	A	1322	C
1	A	1323	G
1	A	1331	G
1	A	1333	A
1	A	1337	G
1	A	1338	G
1	A	1339	A
1	A	1341	U
1	A	1346	A
1	A	1347	G
1	A	1355	G
1	A	1358	U
1	A	1359	C
1	A	1360	A
1	A	1363	C
1	A	1364	U
1	A	1366	C
1	A	1370	G
1	A	1377	A
1	A	1379	G
1	A	1383	C
1	A	1386	G
1	A	1397	C
1	A	1401	G
1	A	1404	C
1	A	1406	U
1	A	1419	G
1	A	1442	G
1	A	1442(A)	G
1	A	1443	G
1	A	1444	C
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	1473	A
1	A	1487	G
1	A	1492	A
1	A	1493	A

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Mol	Chain	Res	Type
1	A	1494	G
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1533	C

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	60	A
1	A	115	G
1	A	119	A
1	A	203	U
1	A	243	A
1	A	266	G
1	A	327	A
1	A	345	C
1	A	428	G
1	A	484	G
1	A	509	A
1	A	560	U
1	A	687	A
1	A	748	C
1	A	840	C
1	A	913	A
1	A	991	U
1	A	992	U
1	A	1064	G
1	A	1065	U
1	A	1067	A
1	A	1201	A
1	A	1211	U
1	A	1285	A
1	A	1300	G
1	A	1442	G

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Mol	Chain	Res	Type
1	A	1493	A
1	A	1504	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 73 ligands modelled in this entry, 73 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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1501/1522 (98%)	0.06	52 (3%) 42 8	53, 112, 168, 181	0
2	B	229/256 (89%)	-0.17	4 (1%) 67 15	113, 135, 150, 160	0
3	C	206/239 (86%)	-0.09	2 (0%) 79 22	119, 140, 153, 162	0
4	D	208/209 (99%)	-0.05	7 (3%) 43 8	95, 111, 129, 142	0
5	E	148/162 (91%)	-0.18	2 (1%) 72 18	87, 108, 124, 132	0
6	F	100/101 (99%)	-0.27	1 (1%) 79 22	93, 107, 123, 135	0
7	G	155/156 (99%)	0.11	9 (5%) 22 5	118, 144, 151, 158	0
8	H	138/138 (100%)	-0.08	0 100 100	89, 110, 120, 133	0
9	I	125/128 (97%)	0.22	6 (4%) 29 6	129, 151, 161, 173	0
10	J	96/105 (91%)	0.08	3 (3%) 47 9	130, 149, 161, 169	0
11	K	114/129 (88%)	-0.17	0 100 100	79, 109, 122, 124	0
12	L	122/132 (92%)	-0.05	1 (0%) 83 26	72, 92, 106, 116	0
13	M	114/126 (90%)	0.25	9 (7%) 13 3	124, 145, 155, 158	0
14	N	60/61 (98%)	0.76	7 (11%) 5 2	136, 146, 152, 155	0
15	O	88/89 (98%)	-0.18	0 100 100	79, 102, 122, 129	0
16	P	82/88 (93%)	0.09	3 (3%) 39 8	89, 105, 123, 132	0
17	Q	99/105 (94%)	-0.15	0 100 100	84, 98, 113, 117	0
18	R	68/88 (77%)	-0.17	1 (1%) 70 16	95, 107, 138, 143	0
19	S	81/93 (87%)	0.33	9 (11%) 6 2	125, 146, 153, 155	0
20	T	97/106 (91%)	-0.02	0 100 100	84, 103, 125, 132	0
21	U	23/27 (85%)	1.85	9 (39%) 1 0	130, 145, 153, 154	0
22	V	53/61 (86%)	-0.46	0 100 100	90, 115, 141, 151	0
All	All	3907/4121 (94%)	0.02	125 (3%) 45 9	53, 118, 159, 181	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1149	C	9.5
1	A	1148	U	7.6
13	M	86	CYS	6.5
1	A	1224	G	6.3
13	M	87	TYR	6.1
19	S	73	GLU	5.9
1	A	1260	C	5.9
7	G	12	LEU	5.6
1	A	1363	C	5.4
21	U	11	GLY	5.3
19	S	74	PHE	5.2
1	A	974	A	5.2
1	A	1125	U	5.0
21	U	6	ARG	4.2
7	G	5	ARG	4.2
7	G	11	GLN	4.2
13	M	85	GLY	3.9
1	A	977	A	3.9
10	J	62	HIS	3.9
9	I	45	ALA	3.8
1	A	389	A	3.8
1	A	915	A	3.8
21	U	4	GLY	3.8
18	R	20	ALA	3.7
19	S	76	PRO	3.7
21	U	3	LYS	3.7
1	A	962	C	3.7
1	A	1150	U	3.7
1	A	1069	C	3.6
2	B	7	VAL	3.6
19	S	69	HIS	3.6
19	S	71	LEU	3.6
1	A	1146	A	3.5
4	D	5	ILE	3.4
4	D	21	LEU	3.4
1	A	743	U	3.3
4	D	23	GLY	3.3
12	L	73	GLU	3.3
9	I	103	THR	3.3
19	S	72	GLY	3.3
21	U	16	GLY	3.3
1	A	1322	C	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	970	C	3.2
21	U	2	GLY	3.2
7	G	13	GLN	3.1
19	S	75	ALA	3.1
1	A	972	C	3.1
1	A	1127	G	3.1
9	I	30	GLY	3.1
21	U	15	ARG	3.0
5	E	81	GLU	3.0
4	D	3	ARG	3.0
1	A	1145	C	3.0
14	N	30	ALA	3.0
13	M	88	ARG	2.9
1	A	1223	C	2.9
1	A	950	U	2.9
21	U	5	ASP	2.9
7	G	4	ARG	2.8
1	A	1147	C	2.8
10	J	100	THR	2.8
1	A	916	G	2.8
1	A	1190	G	2.8
1	A	1394	A	2.8
13	M	90	LEU	2.8
9	I	115	GLY	2.8
1	A	981	U	2.7
1	A	1323	G	2.7
1	A	331	G	2.7
14	N	38	GLY	2.7
3	C	8	ILE	2.7
1	A	1193	G	2.7
1	A	1066	C	2.6
14	N	58	LYS	2.6
7	G	2	ALA	2.6
1	A	971	G	2.6
9	I	66	ARG	2.6
1	A	963	G	2.6
7	G	41	ARG	2.6
1	A	200	G	2.6
1	A	949	A	2.5
7	G	32	ARG	2.5
16	P	10	GLY	2.5
1	A	1324	A	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1332	A	2.5
1	A	1283	G	2.5
1	A	1068	G	2.4
13	M	100	GLY	2.4
9	I	122	ALA	2.4
1	A	223	U	2.4
1	A	1352	C	2.4
1	A	1370	G	2.4
5	E	124	GLY	2.4
4	D	4	TYR	2.4
13	M	58	GLU	2.3
13	M	89	GLY	2.3
21	U	24	ARG	2.3
1	A	1353	G	2.2
13	M	102	ARG	2.2
2	B	161	ALA	2.2
14	N	26	ARG	2.2
14	N	49	HIS	2.2
16	P	76	GLN	2.2
14	N	52	GLN	2.2
3	C	17	ASP	2.2
19	S	36	ARG	2.2
6	F	56	PRO	2.2
1	A	1108	G	2.2
1	A	1124	G	2.2
7	G	108	ALA	2.2
2	B	149	LEU	2.2
1	A	522	C	2.1
19	S	79	THR	2.1
4	D	20	TYR	2.1
1	A	1205	U	2.1
1	A	222	U	2.1
2	B	95	GLN	2.1
1	A	1259	C	2.1
14	N	42	ILE	2.1
4	D	6	GLY	2.1
10	J	99	LYS	2.1
16	P	28	ARG	2.1
1	A	1371	G	2.0
1	A	1286	A	2.0
1	A	742	G	2.0



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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
23	MG	A	1655	1/1	0.09	-	83,83,83,83	0
23	MG	A	1601	1/1	0.39	-	62,62,62,62	0
23	MG	A	1620	1/1	0.51	-	69,69,69,69	0
23	MG	A	1639	1/1	0.19	-	71,71,71,71	0
23	MG	A	1638	1/1	0.49	-	67,67,67,67	0
23	MG	A	1628	1/1	0.14	-	79,79,79,79	0
23	MG	A	1618	1/1	0.12	-	70,70,70,70	0
23	MG	A	1614	1/1	0.28	-	71,71,71,71	0
23	MG	A	1642	1/1	0.39	-	67,67,67,67	0
23	MG	A	1635	1/1	0.09	-	101,101,101,101	0
23	MG	A	1607	1/1	0.22	-	81,81,81,81	0
23	MG	A	1622	1/1	0.14	-	64,64,64,64	0
23	MG	A	1643	1/1	0.29	-	74,74,74,74	0
23	MG	A	1646	1/1	0.32	-	74,74,74,74	0
23	MG	A	1604	1/1	0.22	-	73,73,73,73	0
23	MG	A	1669	1/1	0.07	-	64,64,64,64	0
23	MG	A	1648	1/1	0.32	-	92,92,92,92	0
23	MG	A	1650	1/1	0.10	-	100,100,100,100	0
23	MG	A	1654	1/1	0.20	-	65,65,65,65	0
23	MG	A	1605	1/1	0.24	-	110,110,110,110	0
23	MG	A	1666	1/1	0.14	-	94,94,94,94	0
23	MG	A	1621	1/1	0.21	-	57,57,57,57	0
23	MG	A	1624	1/1	0.48	-	73,73,73,73	0
23	MG	A	1657	1/1	0.28	-	74,74,74,74	0
23	MG	A	1602	1/1	0.18	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
24	ZN	D	301	1/1	0.06	-	96,96,96,96	0
23	MG	A	1608	1/1	0.20	-	72,72,72,72	0
23	MG	A	1611	1/1	0.30	-	80,80,80,80	0
23	MG	A	1656	1/1	0.15	-	95,95,95,95	0
23	MG	A	1658	1/1	0.39	-	97,97,97,97	0
23	MG	A	1668	1/1	0.19	-	131,131,131,131	0
23	MG	A	1609	1/1	0.36	-	67,67,67,67	0
23	MG	A	1665	1/1	0.62	-	91,91,91,91	0
23	MG	A	1651	1/1	0.17	-	92,92,92,92	0
23	MG	A	1627	1/1	0.35	-	86,86,86,86	0
23	MG	A	1663	1/1	0.26	-	100,100,100,100	0
23	MG	A	1660	1/1	0.14	-	83,83,83,83	0
23	MG	A	1616	1/1	0.19	-	76,76,76,76	0
23	MG	A	1636	1/1	0.14	-	68,68,68,68	0
23	MG	A	1633	1/1	0.35	-	65,65,65,65	0
23	MG	A	1625	1/1	0.39	-	82,82,82,82	0
23	MG	A	1603	1/1	0.17	-	82,82,82,82	0
23	MG	A	1667	1/1	0.13	-	76,76,76,76	0
23	MG	A	1626	1/1	0.99	-	88,88,88,88	0
23	MG	A	1610	1/1	0.28	-	70,70,70,70	0
23	MG	A	1659	1/1	0.22	-	86,86,86,86	0
23	MG	A	1617	1/1	0.32	-	72,72,72,72	0
23	MG	A	1623	1/1	0.14	-	74,74,74,74	0
24	ZN	N	101	1/1	0.07	-	188,188,188,188	0
23	MG	A	1613	1/1	0.16	-	84,84,84,84	0
23	MG	A	1629	1/1	0.16	-	55,55,55,55	0
23	MG	A	1649	1/1	0.12	-	78,78,78,78	0
23	MG	A	1661	1/1	0.09	-	60,60,60,60	0
23	MG	A	1652	1/1	0.41	-	100,100,100,100	0
23	MG	A	1612	1/1	0.19	-	64,64,64,64	0
23	MG	A	1653	1/1	0.26	-	61,61,61,61	0
23	MG	A	1632	1/1	0.41	-	88,88,88,88	0
23	MG	A	1619	1/1	0.20	-	75,75,75,75	0
23	MG	A	1662	1/1	0.23	-	106,106,106,106	0
23	MG	A	1647	1/1	0.22	-	63,63,63,63	0
23	MG	A	1615	1/1	0.35	-	69,69,69,69	0
23	MG	A	1640	1/1	0.67	-	61,61,61,61	0
23	MG	A	1631	1/1	0.43	-	72,72,72,72	0
23	MG	A	1641	1/1	0.16	-	62,62,62,62	0
23	MG	A	1606	1/1	0.14	-	74,74,74,74	0
23	MG	A	1637	1/1	0.09	-	77,77,77,77	0
23	MG	A	1671	1/1	0.70	-	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1645	1/1	0.10	-	109,109,109,109	0
23	MG	A	1670	1/1	0.20	-	105,105,105,105	0
23	MG	A	1630	1/1	0.16	-	72,72,72,72	0
23	MG	A	1664	1/1	0.16	-	95,95,95,95	0
23	MG	A	1634	1/1	0.20	-	71,71,71,71	0
23	MG	A	1644	1/1	0.11	-	87,87,87,87	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.