



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 02:07 AM GMT

PDB ID : 3V2E  
Title : Crystal structure of YfiA bound to the 70S ribosome. This PDB entry contains coordinates for the 30S subunit with bound YfiA of the 2nd ribosome in the ASU  
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.  
Deposited on : 2011-12-12  
Resolution : 2.70 Å(reported)

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

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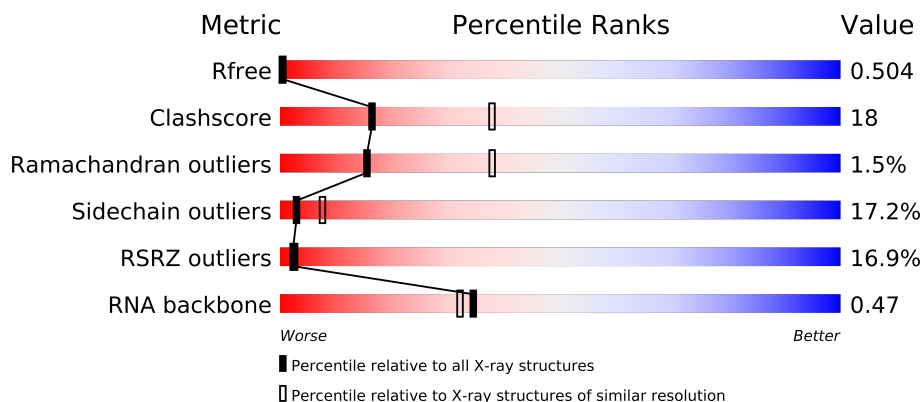
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : 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

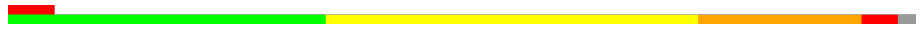

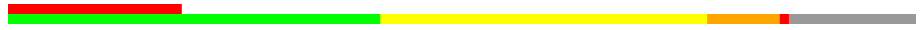









The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)
RNA backbone	1838	1042 (3.20-2.20)

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

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	Y	119	

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 51057 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	1491	Total	C	N	O	P	0	0	0
			32056	14267	5945	10353	1491			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1817	1160	325	327	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
			1453	908	280	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
			1537	968	287	276	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
			1106	700	204	198	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			776	492	135	146	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			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
			1049	667	188	192	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
			849	531	161	157			

- 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
			657	407	129	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	112	Total	C	N	O	S	0	0	0
			784	486	159	138	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
			474	300	98	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
			661	421	126	113	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
			819	525	150	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	78	Total	C	N	O	S	0	0	0
			549	345	106	96	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	104	Total	C	N	O	S	0	0	0
			773	476	162	133	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
			180	112	41	27			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	94	Total	C	N	O	S	0	0	0
			739	461	138	137	3			

There are 6 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	Q	1	Total	Mg	0	0
			1	1		
23	A	208	Total	Mg	0	0
			208	208		
23	E	1	Total	Mg	0	0
			1	1		

- 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	411	Total	O	0	0
			411	411		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	D	2	Total 2	O 2	0	0
25	E	4	Total 4	O 4	0	0
25	F	1	Total 1	O 1	0	0
25	K	1	Total 1	O 1	0	0
25	L	1	Total 1	O 1	0	0
25	P	4	Total 4	O 4	0	0
25	Q	3	Total 3	O 3	0	0
25	R	1	Total 1	O 1	0	0
25	T	2	Total 2	O 2	0	0
25	U	1	Total 1	O 1	0	0

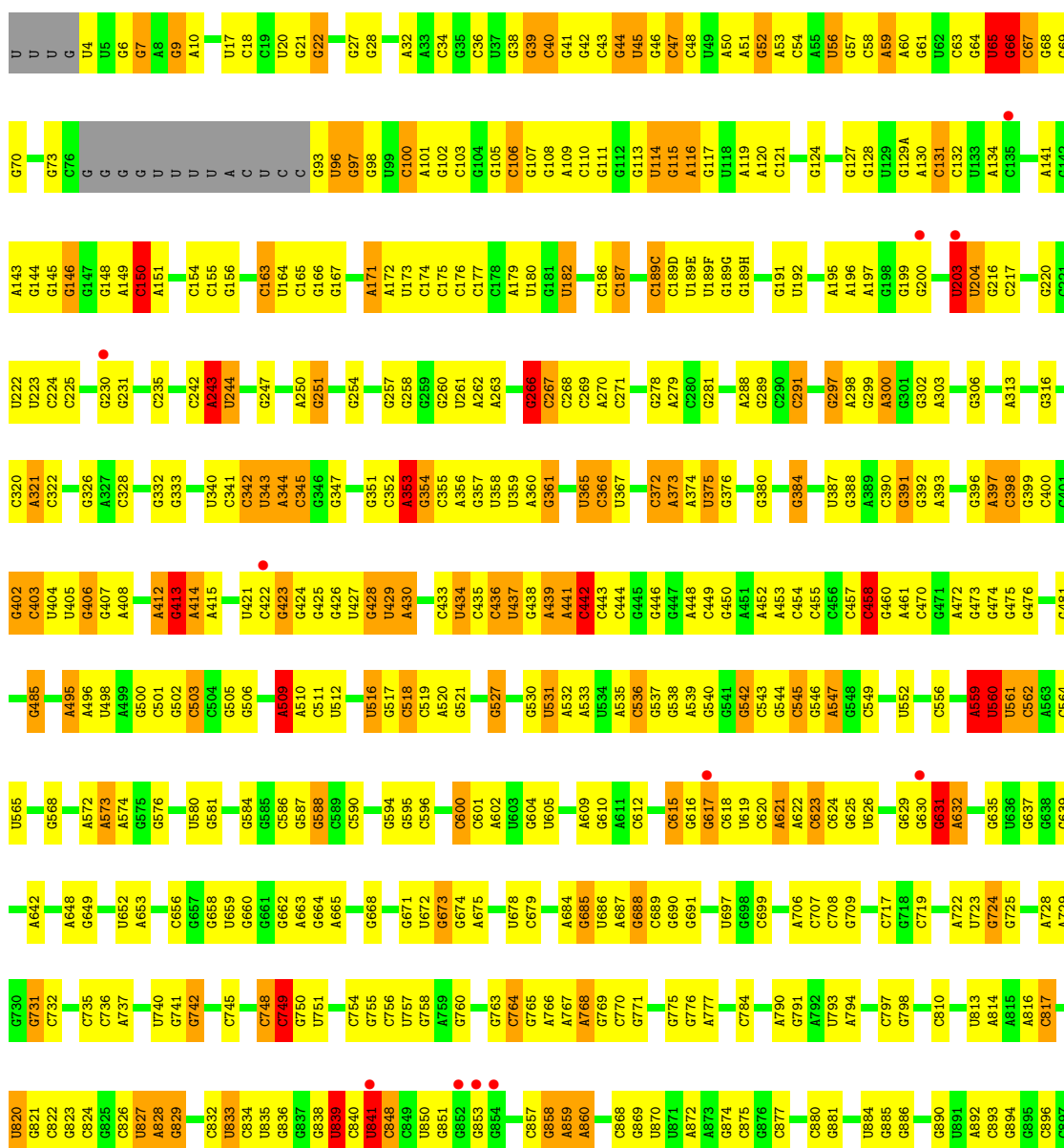


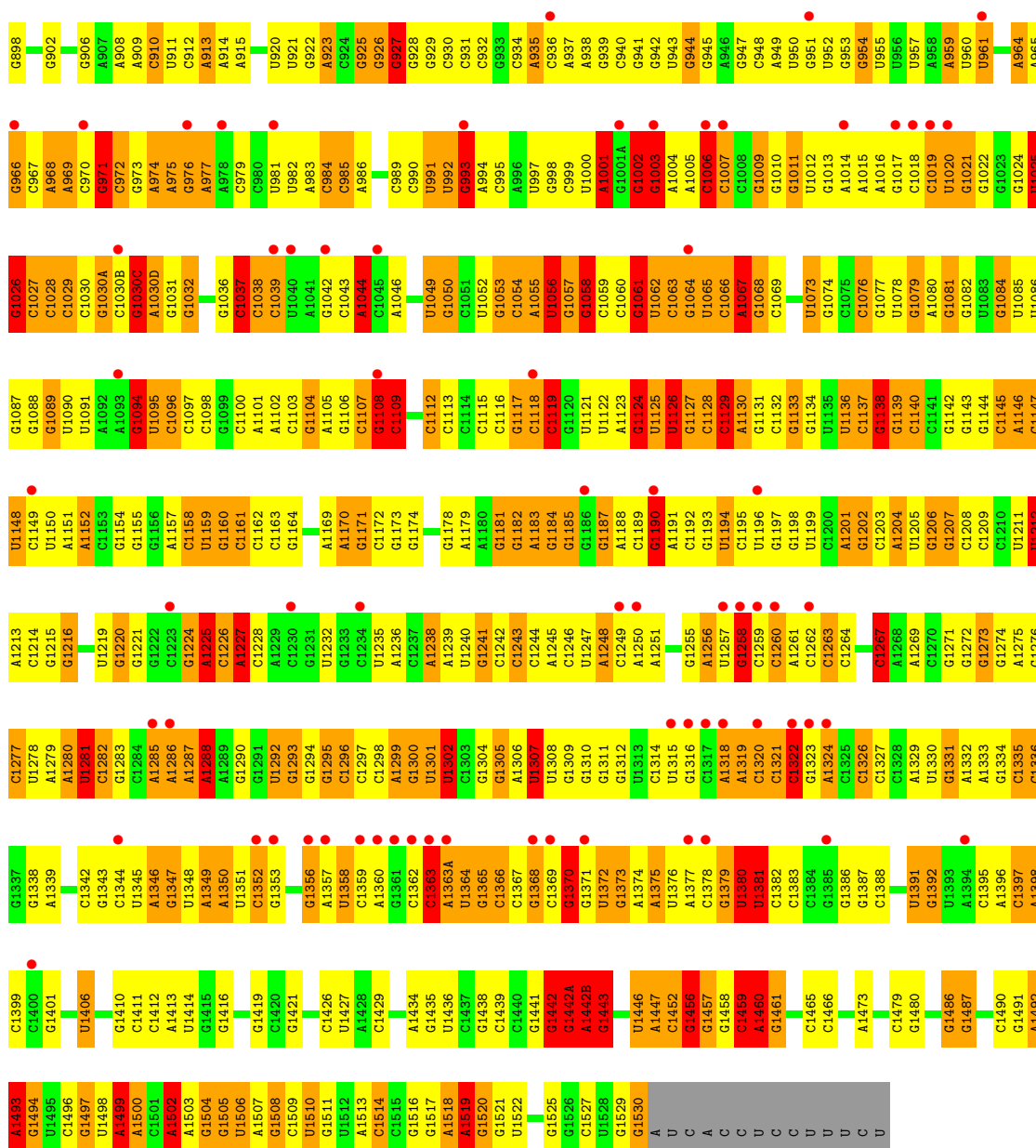
### 3 Residue-property plots

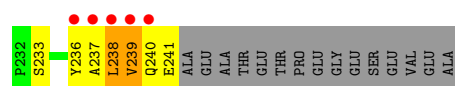
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: 16S Ribosomal RNA

Chain A: 

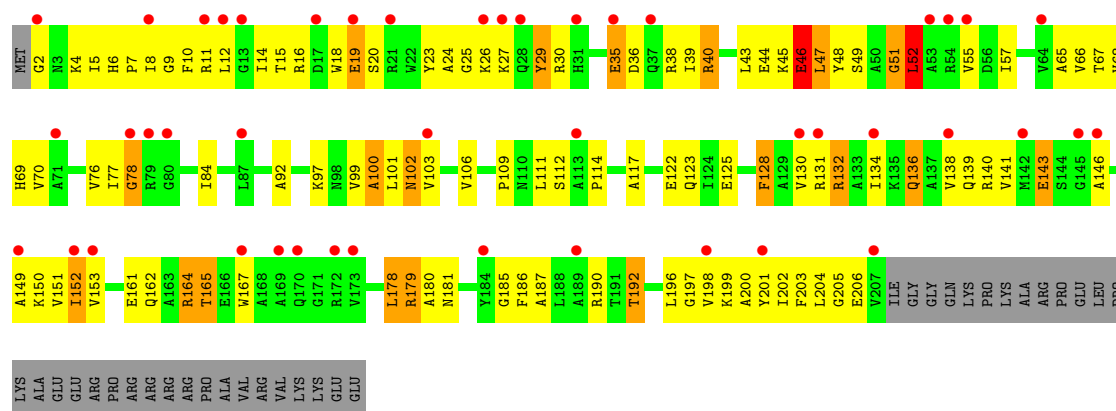






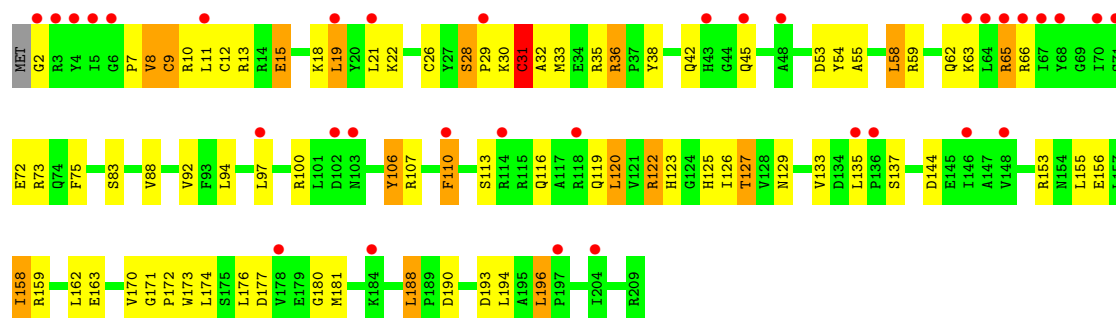
- Molecule 3: 30S Ribosomal Protein S3

Chain C:



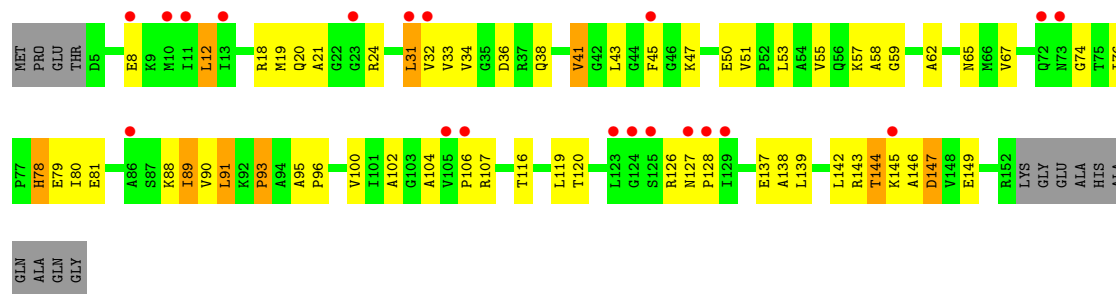
- Molecule 4: 30S Ribosomal Protein S4

Chain D:



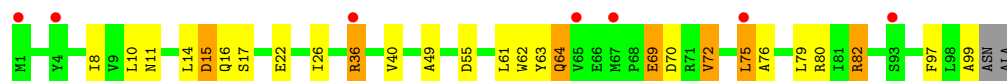
- Molecule 5: 30S Ribosomal Protein S5

Chain E:



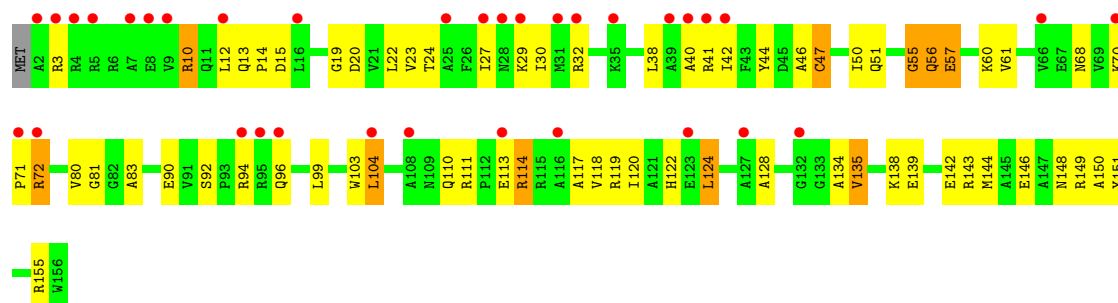
- Molecule 6: 30S Ribosomal Protein S6

Chain F:



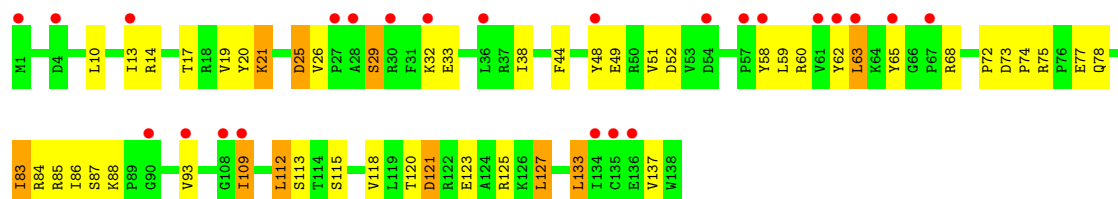
- Molecule 7: 30S Ribosomal Protein S7

Chain G:



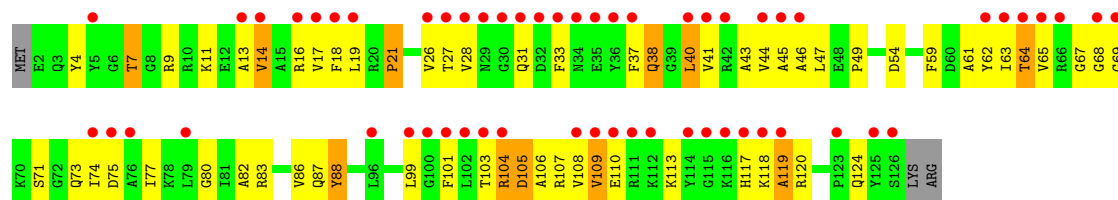
- Molecule 8: 30S Ribosomal Protein S8

Chain H:



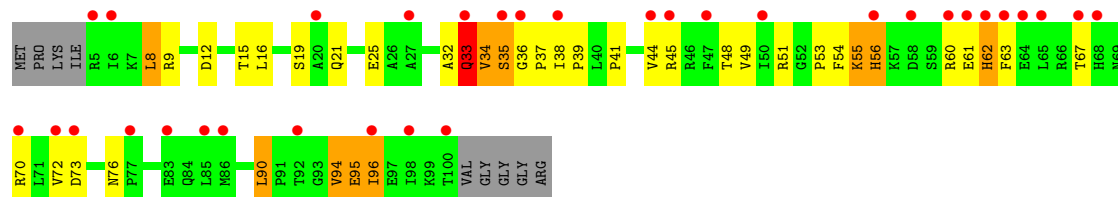
- Molecule 9: 30S Ribosomal Protein S9

Chain I:



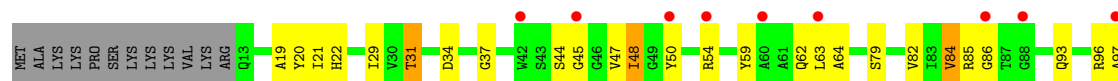
- Molecule 10: 30S Ribosomal Protein S10

Chain J:



- Molecule 11: 30S Ribosomal Protein S11

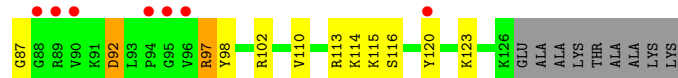
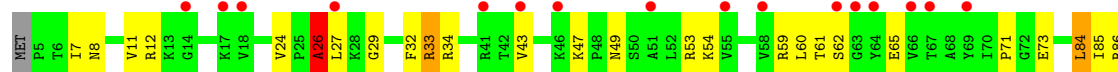
Chain K:





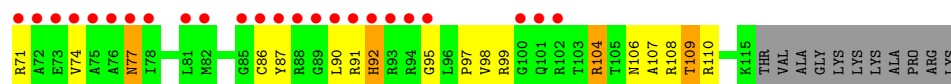
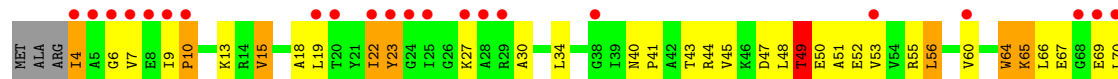
• Molecule 12: 30S Ribosomal Protein S12

Chain L:



• Molecule 13: 30S Ribosomal Protein S13

Chain M:



• Molecule 14: 30S Ribosomal Protein S14

Chain N:



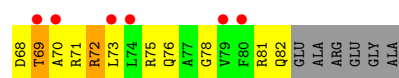
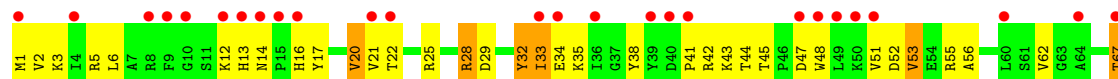
• Molecule 15: 30S Ribosomal Protein S15

Chain O:



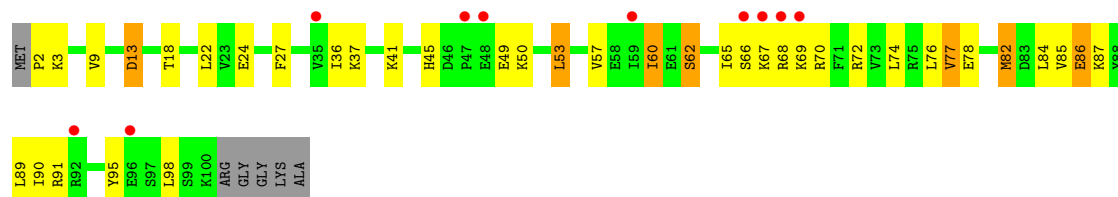
• Molecule 16: 30S Ribosomal Protein S16

Chain P:



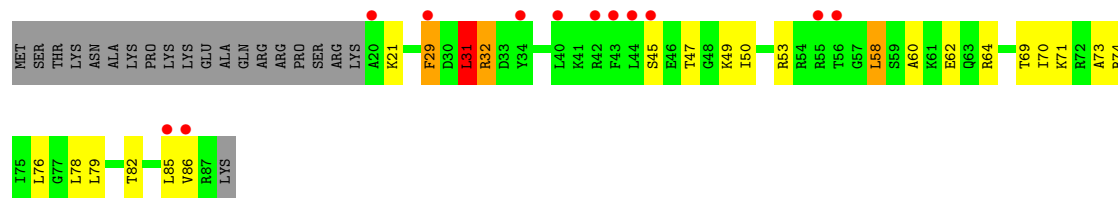
- Molecule 17: 30S Ribosomal Protein S17

Chain Q: 



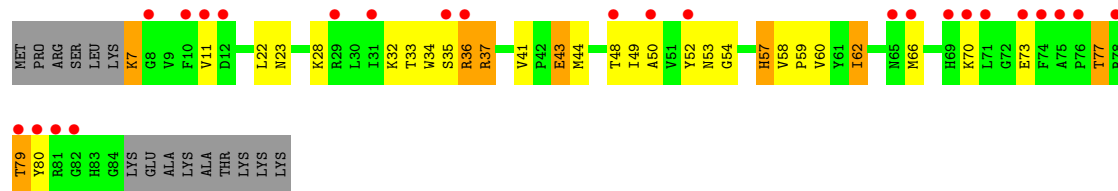
- Molecule 18: 30S Ribosomal Protein S18

Chain R: 



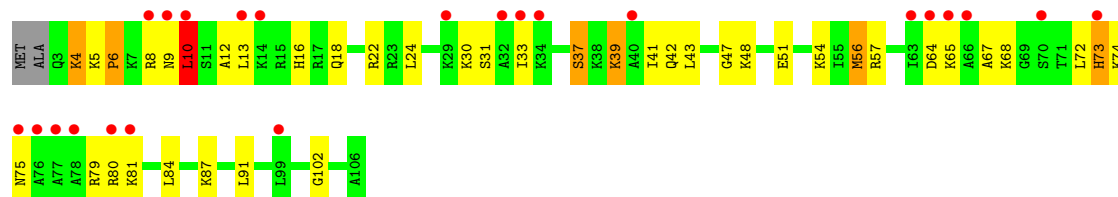
- Molecule 19: 30S Ribosomal Protein S19

Chain S: 



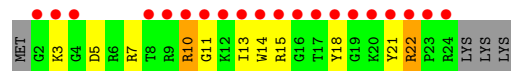
- Molecule 20: 30S Ribosomal Protein S20

Chain T: 



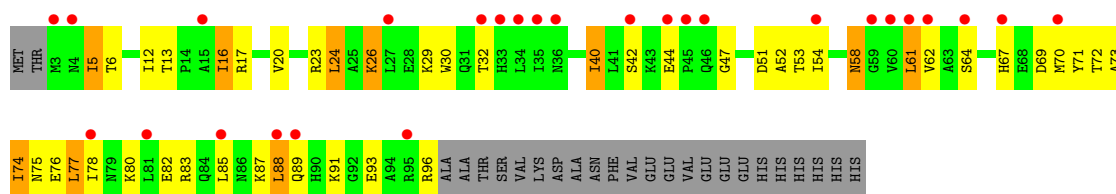
- Molecule 21: 30S Ribosomal Protein THX

Chain U: 



- Molecule 22: Ribosome-associated inhibitor A

Chain Y: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.63Å 449.30Å 620.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.71 – 2.70 49.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.71-2.70) 98.4 (49.71-2.70)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.217 , 0.254 0.503 , 0.504	Depositor DCC
$R_{free}$ test set	78243 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 67.3	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 1557851 reflections	Xtriage
$F_o, F_c$ correlation	0.51	EDS
Total number of atoms	51057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

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

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



## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.97	39/35884 (0.1%)	1.44	557/56006 (1.0%)
2	B	0.62	0/1852	0.75	0/2510
3	C	0.67	0/1477	0.90	4/2006 (0.2%)
4	D	0.68	3/1567 (0.2%)	0.85	1/2125 (0.0%)
5	E	0.64	0/1122	0.81	0/1518
6	F	0.58	0/789	0.78	0/1074
7	G	0.63	0/1183	0.74	0/1599
8	H	0.53	0/1069	0.69	0/1450
9	I	0.70	0/864	0.84	0/1177
10	J	0.73	0/670	0.86	0/917
11	K	0.60	0/843	0.75	0/1144
12	L	0.65	0/921	0.87	2/1247 (0.2%)
13	M	0.72	0/794	0.92	0/1081
14	N	0.68	0/483	0.91	1/645 (0.2%)
15	O	0.57	0/735	0.79	1/981 (0.1%)
16	P	0.57	0/677	0.83	0/917
17	Q	0.62	0/832	0.77	0/1113
18	R	0.52	0/519	0.81	0/699
19	S	0.64	0/563	0.82	0/766
20	T	0.60	0/776	0.83	2/1026 (0.2%)
21	U	0.71	0/184	0.85	0/244
22	Y	0.67	0/751	0.76	0/1017
All	All	0.87	42/54555 (0.1%)	1.28	568/81262 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	3
4	D	0	1
9	I	0	1
10	J	0	2
12	L	0	2
13	M	0	1
14	N	0	2
18	R	0	1
All	All	0	15

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1459	C	N1-C2	17.97	1.58	1.40
1	A	1442(A)	G	N9-C4	15.13	1.50	1.38
1	A	66	G	P-OP2	-12.16	1.28	1.49
1	A	52	G	P-OP1	-11.85	1.28	1.49
1	A	1459	C	C1'-N1	11.46	1.66	1.48
1	A	1459	C	C2-N3	10.41	1.44	1.35
1	A	1442(A)	G	C2-N3	10.12	1.40	1.32
1	A	542	G	P-OP2	-9.51	1.32	1.49
1	A	187	C	P-OP1	-9.48	1.32	1.49
1	A	439	A	P-OP2	-9.37	1.33	1.49
1	A	615	C	P-OP1	-8.98	1.33	1.49
1	A	1442(A)	G	P-OP2	-8.66	1.34	1.49
1	A	439	A	P-OP1	-8.44	1.34	1.49
1	A	44	G	P-OP1	-8.32	1.34	1.49
1	A	542	G	P-OP1	-8.22	1.34	1.49
1	A	516	U	P-OP1	-8.16	1.35	1.49
1	A	615	C	P-OP2	-8.03	1.35	1.49
1	A	187	C	P-OP2	-8.01	1.35	1.49
1	A	341	C	P-OP1	-8.01	1.35	1.49
1	A	1442(A)	G	N3-C4	7.97	1.41	1.35
1	A	341	C	P-OP2	-7.94	1.35	1.49
1	A	516	U	P-OP2	-7.65	1.35	1.49
1	A	1442(A)	G	C5-C6	7.17	1.49	1.42
4	D	12	CYS	CB-SG	7.09	1.94	1.82
1	A	1442(A)	G	P-OP1	-7.08	1.36	1.49
4	D	9	CYS	CB-SG	7.02	1.94	1.82
1	A	44	G	P-OP2	-6.97	1.37	1.49
4	D	31	CYS	CB-SG	-6.63	1.71	1.82
1	A	1003	G	N9-C4	6.43	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	398	C	N3-C4	-6.35	1.29	1.33
1	A	1067	A	N9-C4	6.26	1.41	1.37
1	A	65	U	C3'-O3'	5.96	1.50	1.42
1	A	47	C	C2-N3	-5.90	1.31	1.35
1	A	1493	A	N9-C4	5.54	1.41	1.37
1	A	52	G	P-O5'	-5.50	1.54	1.59
1	A	1442(A)	G	C6-N1	5.30	1.43	1.39
1	A	1030(D)	A	N9-C4	5.28	1.41	1.37
1	A	1525	G	N7-C5	5.24	1.42	1.39
1	A	1124	G	N9-C4	5.21	1.42	1.38
1	A	1446	U	N1-C2	5.21	1.43	1.38
1	A	1036	G	N9-C4	5.20	1.42	1.38
1	A	44	G	N9-C4	-5.15	1.33	1.38

All (568) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1459	C	C6-N1-C2	-31.40	107.74	120.30
1	A	1459	C	N3-C2-O2	-28.90	101.67	121.90
1	A	1442(A)	G	N3-C4-C5	-25.05	116.07	128.60
1	A	1459	C	N1-C2-O2	20.36	131.12	118.90
1	A	1442(A)	G	C6-N1-C2	-19.04	113.68	125.10
1	A	1442(A)	G	N3-C4-N9	18.02	136.81	126.00
1	A	1442(A)	G	C2-N3-C4	17.90	120.85	111.90
1	A	1442(A)	G	C5-C6-N1	17.75	120.37	111.50
1	A	1459	C	C2-N1-C1'	17.71	138.28	118.80
1	A	44	G	N1-C6-O6	14.99	128.89	119.90
1	A	361	G	N1-C6-O6	12.94	127.67	119.90
1	A	1442(B)	A	N1-C2-N3	12.83	135.71	129.30
1	A	47	C	C6-N1-C2	12.50	125.30	120.30
1	A	1442(A)	G	C8-N9-C4	-12.38	101.45	106.40
1	A	1442(A)	G	C4-N9-C1'	11.86	141.92	126.50
1	A	1158	C	C6-N1-C2	-11.79	115.58	120.30
1	A	1391	U	C5-C4-O4	11.64	132.88	125.90
1	A	1459	C	C2-N3-C4	-11.61	114.09	119.90
1	A	1459	C	N1-C2-N3	11.44	127.21	119.20
1	A	365	U	C5-C6-N1	-11.44	116.98	122.70
1	A	1459	C	C5-C6-N1	11.33	126.66	121.00
1	A	1003	G	C2-N3-C4	10.64	117.22	111.90
1	A	1003	G	N3-C4-C5	-10.62	123.29	128.60
1	A	1267	C	C2-N1-C1'	10.62	130.48	118.80
1	A	44	G	C5-C6-N1	-10.61	106.20	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	C	C6-N1-C2	10.53	124.51	120.30
1	A	39	G	C6-N1-C2	-10.50	118.80	125.10
1	A	40	C	C2-N3-C4	-10.40	114.70	119.90
1	A	44	G	C6-N1-C2	10.10	131.16	125.10
1	A	1260	C	C6-N1-C2	-10.00	116.30	120.30
1	A	403	C	C2-N3-C4	-9.90	114.95	119.90
1	A	1460	A	C5-N7-C8	9.84	108.82	103.90
1	A	398	C	C2-N3-C4	9.46	124.63	119.90
1	A	39	G	N1-C6-O6	-9.40	114.26	119.90
1	A	1443	G	C5-C6-N1	9.40	116.20	111.50
1	A	44	G	N3-C4-C5	9.21	133.20	128.60
1	A	303	A	C8-N9-C4	9.18	109.47	105.80
1	A	1442	G	C5-N7-C8	9.09	108.85	104.30
1	A	1460	A	N1-C6-N6	-9.05	113.17	118.60
1	A	358	U	C2-N3-C4	-9.04	121.57	127.00
1	A	1067	A	C8-N9-C4	-8.88	102.25	105.80
1	A	53	A	N1-C6-N6	-8.82	113.31	118.60
1	A	913	A	C8-N9-C4	-8.78	102.29	105.80
1	A	839	U	N1-C2-O2	8.76	128.93	122.80
1	A	1460	A	N7-C8-N9	-8.64	109.48	113.80
1	A	358	U	N1-C2-N3	8.59	120.06	114.90
1	A	366	C	C5-C6-N1	-8.58	116.71	121.00
1	A	1009	G	C5-C6-O6	8.53	133.72	128.60
1	A	365	U	C2-N1-C1'	-8.52	107.47	117.70
1	A	1205	U	C6-N1-C2	-8.47	115.92	121.00
1	A	1459	C	C4-C5-C6	8.41	121.60	117.40
1	A	1442(A)	G	C8-N9-C1'	-8.38	116.11	127.00
1	A	44	G	C2-N3-C4	-8.27	107.76	111.90
1	A	402	G	C6-N1-C2	-8.27	120.14	125.10
1	A	1030(A)	G	C8-N9-C4	-8.25	103.10	106.40
1	A	1442(A)	G	C5-C6-O6	-8.25	123.65	128.60
1	A	1366	C	N1-C2-O2	8.18	123.81	118.90
1	A	1181	G	C4-N9-C1'	-8.15	115.90	126.50
1	A	1442	G	C4-C5-N7	-8.14	107.54	110.80
1	A	1442(A)	G	N1-C2-N2	-8.11	108.90	116.20
1	A	357	G	N1-C6-O6	-8.06	115.06	119.90
1	A	297	G	N1-C6-O6	8.02	124.71	119.90
1	A	1486	G	N1-C6-O6	8.02	124.71	119.90
1	A	45	U	N3-C2-O2	8.00	127.80	122.20
1	A	47	C	C2-N1-C1'	-7.99	110.01	118.80
1	A	1258	G	N3-C2-N2	7.98	125.49	119.90
1	A	1518	A	C5-C6-N6	7.98	130.08	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	C	C6-N1-C2	-7.96	117.12	120.30
1	A	1321	C	C6-N1-C2	-7.95	117.12	120.30
1	A	403	C	N3-C2-O2	-7.93	116.35	121.90
3	C	52	LEU	CA-CB-CG	7.92	133.50	115.30
1	A	1206	G	N3-C4-N9	7.91	130.74	126.00
1	A	1003	G	C8-N9-C4	-7.90	103.24	106.40
1	A	1006	C	C5-C6-N1	7.90	124.95	121.00
1	A	1267	C	C5-C6-N1	7.86	124.93	121.00
1	A	399	G	N1-C6-O6	7.85	124.61	119.90
1	A	39	G	C5-C6-N1	7.84	115.42	111.50
1	A	299	G	C2-N3-C4	-7.80	108.00	111.90
1	A	893	C	C6-N1-C2	7.75	123.40	120.30
1	A	509	A	C8-N9-C4	-7.69	102.72	105.80
1	A	1502	A	N1-C2-N3	7.69	133.14	129.30
1	A	1029	C	C6-N1-C2	-7.67	117.23	120.30
1	A	1443	G	N1-C6-O6	-7.66	115.31	119.90
1	A	365	U	N3-C4-O4	-7.64	114.05	119.40
1	A	53	A	C6-N1-C2	-7.61	114.03	118.60
1	A	925	G	C8-N9-C4	7.61	109.44	106.40
1	A	40	C	N3-C2-O2	-7.60	116.58	121.90
1	A	1267	C	C6-N1-C1'	-7.57	111.71	120.80
1	A	893	C	N1-C2-O2	7.56	123.44	118.90
1	A	1381	U	N3-C2-O2	-7.51	116.94	122.20
1	A	300	A	C6-N1-C2	-7.49	114.11	118.60
1	A	365	U	C5-C4-O4	7.48	130.38	125.90
1	A	413	G	C4-C5-N7	-7.46	107.81	110.80
1	A	1126	U	C5-C6-N1	7.46	126.43	122.70
1	A	912	C	C5-C6-N1	-7.46	117.27	121.00
4	D	12	CYS	CA-CB-SG	7.44	127.39	114.00
1	A	1181	G	C8-N9-C1'	7.39	136.61	127.00
1	A	722	A	N1-C6-N6	7.39	123.03	118.60
1	A	1370	G	C8-N9-C4	-7.35	103.46	106.40
1	A	365	U	N1-C2-N3	7.34	119.30	114.90
1	A	47	C	N1-C2-N3	-7.33	114.07	119.20
1	A	396	G	N1-C6-O6	7.31	124.29	119.90
1	A	896	C	C6-N1-C2	7.31	123.23	120.30
1	A	1322	C	C6-N1-C2	-7.30	117.38	120.30
1	A	1456	G	C4-N9-C1'	-7.25	117.07	126.50
1	A	1267	C	N1-C2-O2	7.23	123.24	118.90
1	A	1391	U	N3-C4-O4	-7.23	114.34	119.40
1	A	1443	G	C4-C5-C6	-7.22	114.47	118.80
1	A	1504	G	C4-N9-C1'	-7.22	117.12	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1277	C	C2-N3-C4	7.21	123.50	119.90
1	A	1504	G	C8-N9-C4	7.21	109.28	106.40
1	A	365	U	C2-N3-C4	-7.20	122.68	127.00
1	A	403	C	N3-C4-C5	7.18	124.77	121.90
14	N	13	THR	C-N-CD	-7.17	104.84	120.60
1	A	910	C	N1-C2-O2	-7.15	114.61	118.90
1	A	1081	G	C8-N9-C4	7.14	109.26	106.40
1	A	1089	G	N9-C4-C5	7.12	108.25	105.40
1	A	361	G	C5-C6-N1	-7.11	107.95	111.50
1	A	1281	U	C5-C6-N1	7.11	126.25	122.70
1	A	1502	A	C2-N3-C4	-7.11	107.05	110.60
1	A	1119	C	C6-N1-C2	-7.10	117.46	120.30
1	A	824	C	C2-N1-C1'	-7.09	111.00	118.80
1	A	361	G	C6-N1-C2	7.05	129.33	125.10
1	A	1502	A	N7-C8-N9	7.04	117.32	113.80
1	A	1077	G	C8-N9-C4	7.03	109.21	106.40
1	A	361	G	C5-C6-O6	-7.02	124.39	128.60
1	A	1293	G	C4-C5-N7	-7.02	107.99	110.80
1	A	40	C	N3-C4-C5	7.02	124.71	121.90
1	A	1502	A	C5-N7-C8	-7.01	100.40	103.90
1	A	1216	G	C8-N9-C4	7.00	109.20	106.40
1	A	1061	G	N3-C4-C5	-6.99	125.10	128.60
1	A	770	C	C6-N1-C2	6.99	123.09	120.30
1	A	1079	G	C8-N9-C4	-6.98	103.61	106.40
1	A	1486	G	C5-C6-O6	-6.95	124.43	128.60
1	A	925	G	C5-C6-O6	-6.95	124.43	128.60
1	A	1158	C	C2-N1-C1'	6.94	126.44	118.80
1	A	839	U	N3-C2-O2	-6.93	117.35	122.20
1	A	1442	G	N7-C8-N9	-6.92	109.64	113.10
1	A	1322	C	N3-C4-C5	-6.89	119.14	121.90
1	A	1096	C	C6-N1-C1'	6.87	129.04	120.80
1	A	1076	C	N3-C4-C5	6.87	124.65	121.90
1	A	1460	A	C6-C5-N7	6.85	137.09	132.30
1	A	27	G	C5-C6-O6	-6.83	124.50	128.60
1	A	1442(B)	A	C2-N3-C4	-6.83	107.19	110.60
1	A	1514	C	N1-C2-O2	-6.82	114.81	118.90
1	A	1527	C	C6-N1-C2	6.81	123.02	120.30
1	A	1381	U	N1-C2-O2	6.79	127.56	122.80
1	A	266	G	C5-N7-C8	-6.78	100.91	104.30
1	A	560	U	C2-N1-C1'	6.78	125.83	117.70
1	A	1044	A	C5-C6-N6	6.76	129.10	123.70
1	A	266	G	C2-N3-C4	-6.75	108.53	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	G	N1-C2-N2	-6.74	110.13	116.20
1	A	945	G	N1-C6-O6	6.73	123.94	119.90
1	A	839	U	C2-N1-C1'	6.72	125.77	117.70
1	A	396	G	C6-N1-C2	6.71	129.13	125.10
1	A	1076	C	C6-N1-C2	6.70	122.98	120.30
1	A	890	G	C8-N9-C4	6.70	109.08	106.40
1	A	1504	G	N3-C4-C5	6.70	131.95	128.60
1	A	836	G	N1-C6-O6	6.69	123.91	119.90
1	A	1020	U	C2-N3-C4	-6.68	122.99	127.00
1	A	1307	U	C5-C6-N1	6.68	126.04	122.70
1	A	927	G	N1-C6-O6	-6.67	115.90	119.90
1	A	1056	U	C2-N3-C4	6.66	131.00	127.00
1	A	1460	A	C4-C5-N7	-6.65	107.37	110.70
1	A	495	A	N1-C6-N6	-6.62	114.63	118.60
1	A	1395	C	N3-C4-C5	-6.62	119.25	121.90
1	A	54	C	N3-C2-O2	-6.62	117.27	121.90
20	T	10	LEU	CA-CB-CG	6.62	130.52	115.30
1	A	1029	C	C5-C6-N1	6.62	124.31	121.00
1	A	817	C	N1-C2-O2	-6.61	114.93	118.90
1	A	53	A	N1-C2-N3	6.61	132.61	129.30
1	A	1397	C	C2-N1-C1'	6.61	126.06	118.80
1	A	150	C	C5-C6-N1	6.60	124.30	121.00
1	A	1442(A)	G	N1-C6-O6	-6.60	115.94	119.90
1	A	1293	G	N9-C4-C5	6.59	108.04	105.40
1	A	481	G	N3-C4-C5	-6.59	125.31	128.60
1	A	1148	U	C5-C4-O4	-6.58	121.95	125.90
1	A	44	G	N3-C4-N9	-6.57	122.06	126.00
1	A	1057	G	C8-N9-C4	6.56	109.03	106.40
1	A	968	A	N1-C6-N6	6.56	122.54	118.60
1	A	1145	C	C2-N3-C4	6.55	123.17	119.90
1	A	912	C	C6-N1-C2	6.54	122.92	120.30
1	A	850	U	C5-C4-O4	6.53	129.82	125.90
1	A	361	G	C6-C5-N7	-6.52	126.49	130.40
1	A	1003	G	N3-C4-N9	6.52	129.91	126.00
1	A	372	C	N1-C2-O2	6.52	122.81	118.90
1	A	1096	C	N1-C2-O2	-6.50	115.00	118.90
1	A	1108	G	C5-C6-O6	6.50	132.50	128.60
1	A	1499	A	C8-N9-C4	6.49	108.39	105.80
1	A	1002	G	C8-N9-C4	-6.47	103.81	106.40
1	A	1356	G	C8-N9-C4	-6.45	103.82	106.40
1	A	1446	U	N1-C2-O2	6.44	127.31	122.80
20	T	10	LEU	N-CA-C	6.43	128.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	C	C6-N1-C2	6.43	122.87	120.30
1	A	442	C	C6-N1-C2	-6.42	117.73	120.30
1	A	732	C	C5-C6-N1	-6.42	117.79	121.00
1	A	266	G	N3-C4-C5	6.41	131.80	128.60
1	A	925	G	N7-C8-N9	-6.40	109.90	113.10
1	A	399	G	C5-C6-O6	-6.40	124.76	128.60
1	A	1442(A)	G	N3-C2-N2	6.38	124.37	119.90
1	A	43	C	N3-C2-O2	6.37	126.36	121.90
1	A	699	C	C6-N1-C2	-6.36	117.76	120.30
1	A	1129	C	C6-N1-C2	-6.36	117.76	120.30
1	A	358	U	N3-C4-O4	-6.34	114.96	119.40
1	A	1067	A	N7-C8-N9	6.32	116.96	113.80
1	A	47	C	N3-C2-O2	6.32	126.32	121.90
1	A	303	A	N7-C8-N9	-6.32	110.64	113.80
1	A	927	G	C5-C6-O6	6.32	132.39	128.60
1	A	1158	C	N3-C2-O2	-6.32	117.48	121.90
1	A	1527	C	C5-C6-N1	-6.31	117.84	121.00
1	A	1001	A	C8-N9-C4	-6.31	103.28	105.80
1	A	912	C	C4-C5-C6	6.31	120.56	117.40
1	A	1372	U	C6-N1-C2	-6.30	117.22	121.00
1	A	1395	C	C2-N3-C4	6.30	123.05	119.90
1	A	1030(A)	G	N9-C4-C5	6.30	107.92	105.40
1	A	1100	C	C2-N1-C1'	-6.30	111.87	118.80
1	A	281	G	C8-N9-C4	-6.29	103.89	106.40
1	A	1006	C	C2-N3-C4	6.29	123.04	119.90
1	A	27	G	N1-C6-O6	6.27	123.66	119.90
1	A	47	C	C4-C5-C6	-6.27	114.27	117.40
1	A	1020	U	N1-C2-N3	6.26	118.66	114.90
1	A	28	G	C8-N9-C4	-6.26	103.90	106.40
1	A	353	A	N7-C8-N9	6.26	116.93	113.80
1	A	288	A	C2-N3-C4	-6.26	107.47	110.60
1	A	824	C	N1-C2-O2	-6.23	115.16	118.90
1	A	1373	G	C8-N9-C4	-6.23	103.91	106.40
1	A	1267	C	C6-N1-C2	-6.23	117.81	120.30
1	A	1373	G	N3-C4-C5	-6.21	125.49	128.60
1	A	1442(A)	G	N7-C8-N9	6.20	116.20	113.10
1	A	971	G	C8-N9-C4	6.20	108.88	106.40
1	A	1292	U	C6-N1-C2	6.20	124.72	121.00
1	A	413	G	C5-C6-O6	6.18	132.31	128.60
1	A	824	C	C6-N1-C2	6.18	122.77	120.30
1	A	1069	C	C6-N1-C2	-6.18	117.83	120.30
1	A	1260	C	C5-C6-N1	6.17	124.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189(C)	C	C6-N1-C2	-6.16	117.83	120.30
1	A	1514	C	N3-C4-C5	-6.16	119.44	121.90
1	A	44	G	C5-C6-O6	-6.16	124.90	128.60
1	A	1158	C	C5-C6-N1	6.15	124.08	121.00
1	A	361	G	C4-C5-N7	6.15	113.26	110.80
1	A	925	G	N3-C4-N9	6.15	129.69	126.00
1	A	881	G	N1-C6-O6	-6.15	116.21	119.90
1	A	912	C	C2-N1-C1'	-6.14	112.04	118.80
1	A	1320	C	C6-N1-C2	-6.13	117.85	120.30
1	A	356	A	C6-N1-C2	-6.13	114.92	118.60
1	A	881	G	C5-C6-O6	6.13	132.28	128.60
1	A	1290	G	C8-N9-C4	-6.13	103.95	106.40
1	A	929	G	C8-N9-C4	-6.11	103.95	106.40
1	A	1352	C	N3-C4-C5	-6.10	119.46	121.90
1	A	458	C	N3-C4-C5	-6.09	119.47	121.90
1	A	1205	U	C5-C6-N1	6.08	125.74	122.70
1	A	1190	G	C8-N9-C4	6.08	108.83	106.40
1	A	1181	G	N3-C4-N9	-6.07	122.36	126.00
1	A	1096	C	C6-N1-C2	-6.07	117.87	120.30
1	A	754	C	N1-C2-O2	6.06	122.54	118.90
1	A	117	G	C5-C6-O6	-6.06	124.97	128.60
1	A	1100	C	C6-N1-C1'	6.05	128.06	120.80
1	A	913	A	N9-C4-C5	6.05	108.22	105.80
1	A	1375	A	C8-N9-C4	-6.05	103.38	105.80
1	A	365	U	C6-N1-C1'	6.04	129.65	121.20
1	A	745	C	C6-N1-C2	-6.03	117.89	120.30
1	A	1460	A	C5-C6-N6	6.00	128.50	123.70
1	A	1350	A	C5-C6-N6	6.00	128.50	123.70
1	A	1356	G	N7-C8-N9	6.00	116.10	113.10
1	A	1277	C	C6-N1-C2	-5.98	117.91	120.30
1	A	740	U	C5-C6-N1	-5.98	119.71	122.70
1	A	1442(B)	A	C5-C6-N6	5.97	128.48	123.70
1	A	1006	C	N1-C2-O2	5.96	122.48	118.90
1	A	1094	G	N3-C4-N9	5.96	129.57	126.00
1	A	52	G	N1-C6-O6	-5.95	116.33	119.90
1	A	413	G	N3-C4-N9	-5.95	122.43	126.00
1	A	964	A	C8-N9-C4	-5.95	103.42	105.80
1	A	1399	C	N3-C4-N4	5.94	122.16	118.00
1	A	398	C	N3-C2-O2	5.94	126.06	121.90
1	A	697	U	C6-N1-C2	5.94	124.56	121.00
1	A	1518	A	C5-C6-N1	-5.93	114.73	117.70
1	A	1380	U	N1-C2-O2	5.92	126.94	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1366	C	N3-C2-O2	-5.91	117.77	121.90
1	A	63	C	C6-N1-C2	-5.90	117.94	120.30
1	A	1392	G	C8-N9-C4	5.89	108.76	106.40
1	A	41	G	C8-N9-C4	-5.88	104.05	106.40
1	A	171	A	C8-N9-C4	-5.88	103.45	105.80
1	A	39	G	N1-C2-N3	5.88	127.43	123.90
1	A	436	C	C6-N1-C2	5.87	122.65	120.30
1	A	1395	C	C6-N1-C2	-5.87	117.95	120.30
1	A	1522	U	C4-C5-C6	5.87	123.22	119.70
1	A	972	C	C6-N1-C2	-5.87	117.95	120.30
1	A	1500	A	C2-N3-C4	-5.87	107.67	110.60
1	A	356	A	C5-C6-N1	5.86	120.63	117.70
1	A	810	C	C6-N1-C2	5.85	122.64	120.30
1	A	1267	C	C2-N3-C4	5.85	122.83	119.90
1	A	423	G	N3-C4-N9	5.85	129.51	126.00
1	A	1296	C	C2-N1-C1'	5.83	125.22	118.80
1	A	1520	G	C8-N9-C4	5.83	108.73	106.40
1	A	400	C	C2-N3-C4	5.82	122.81	119.90
1	A	396	G	C5-C6-N1	-5.82	108.59	111.50
3	C	78	GLY	N-CA-C	5.81	127.64	113.10
1	A	1204	A	C6-N1-C2	5.81	122.08	118.60
1	A	1522	U	N1-C2-N3	5.80	118.38	114.90
1	A	42	G	N1-C6-O6	5.80	123.38	119.90
1	A	65	U	P-O3'-C3'	5.79	126.65	119.70
1	A	1009	G	C6-N1-C2	5.79	128.57	125.10
1	A	355	C	N3-C2-O2	-5.78	117.85	121.90
1	A	997	U	C5-C4-O4	5.78	129.37	125.90
1	A	1281	U	C6-N1-C2	-5.77	117.54	121.00
1	A	1442(A)	G	C4-C5-C6	5.76	122.25	118.80
1	A	366	C	N3-C4-C5	5.75	124.20	121.90
1	A	1225	A	N7-C8-N9	5.75	116.67	113.80
1	A	402	G	N3-C4-C5	-5.75	125.73	128.60
1	A	1363	C	C2-N1-C1'	-5.75	112.48	118.80
1	A	754	C	C2-N1-C1'	5.74	125.11	118.80
1	A	810	C	C5-C6-N1	-5.74	118.13	121.00
1	A	928	G	N1-C6-O6	5.74	123.34	119.90
1	A	1292	U	C5-C6-N1	-5.74	119.83	122.70
1	A	402	G	C5-C6-N1	5.74	114.37	111.50
1	A	436	C	C6-N1-C1'	-5.73	113.93	120.80
1	A	568	G	C8-N9-C4	-5.72	104.11	106.40
1	A	56	U	C2-N3-C4	-5.72	123.57	127.00
1	A	358	U	N3-C2-O2	-5.71	118.20	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1044	A	C6-N1-C2	5.71	122.03	118.60
15	O	17	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	278	G	N3-C2-N2	-5.71	115.90	119.90
1	A	1104	G	N3-C4-C5	-5.71	125.75	128.60
1	A	1129	C	N1-C2-O2	5.71	122.32	118.90
3	C	51	GLY	C-N-CA	5.71	135.96	121.70
1	A	1518	A	N1-C6-N6	-5.70	115.18	118.60
1	A	1089	G	C4-C5-N7	-5.70	108.52	110.80
1	A	1158	C	N3-C4-C5	-5.70	119.62	121.90
1	A	1459	C	C6-N1-C1'	-5.70	113.96	120.80
1	A	400	C	N1-C2-N3	-5.70	115.21	119.20
1	A	1030(C)	G	C8-N9-C4	-5.70	104.12	106.40
1	A	823	G	C8-N9-C4	5.70	108.68	106.40
1	A	836	G	C5-C6-O6	-5.70	125.18	128.60
1	A	1370	G	N7-C8-N9	5.69	115.94	113.10
1	A	400	C	C6-N1-C2	5.69	122.58	120.30
1	A	1207	G	N3-C4-N9	-5.68	122.59	126.00
1	A	357	G	C6-N1-C2	-5.67	121.70	125.10
1	A	927	G	C8-N9-C4	-5.67	104.13	106.40
1	A	1006	C	C4-C5-C6	-5.67	114.56	117.40
1	A	893	C	N3-C4-C5	5.67	124.17	121.90
1	A	1443	G	C4-N9-C1'	-5.67	119.13	126.50
1	A	1521	G	C8-N9-C4	-5.67	104.13	106.40
1	A	357	G	C4-C5-N7	-5.65	108.54	110.80
1	A	1518	A	C4-C5-N7	-5.63	107.88	110.70
1	A	1349	A	N1-C6-N6	5.63	121.98	118.60
1	A	42	G	C5-C6-N1	-5.63	108.69	111.50
1	A	345	C	N3-C4-C5	5.63	124.15	121.90
1	A	1227	A	C2-N3-C4	-5.63	107.79	110.60
1	A	43	C	N1-C2-O2	-5.62	115.53	118.90
1	A	927	G	N9-C4-C5	5.62	107.65	105.40
1	A	1364	U	C6-N1-C2	-5.62	117.62	121.00
1	A	754	C	N3-C2-O2	-5.62	117.97	121.90
1	A	1181	G	N3-C2-N2	-5.61	115.97	119.90
1	A	1510	U	C6-N1-C2	5.61	124.37	121.00
1	A	1108	G	C4-C5-N7	-5.61	108.56	110.80
1	A	100	C	C6-N1-C2	-5.61	118.06	120.30
1	A	40	C	N3-C4-N4	-5.60	114.08	118.00
1	A	1366	C	C2-N3-C4	5.60	122.70	119.90
1	A	1003	G	C4-N9-C1'	5.60	133.78	126.50
1	A	322	C	N3-C2-O2	5.59	125.82	121.90
1	A	1112	C	C6-N1-C2	-5.58	118.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1443	G	C8-N9-C4	5.58	108.63	106.40
1	A	340	U	C6-N1-C2	5.58	124.34	121.00
1	A	1519	A	C8-N9-C4	-5.57	103.57	105.80
1	A	925	G	C6-N1-C2	-5.57	121.76	125.10
1	A	932	C	C6-N1-C2	-5.57	118.07	120.30
1	A	1044	A	N1-C6-N6	-5.57	115.26	118.60
1	A	356	A	C2-N3-C4	5.56	113.38	110.60
1	A	945	G	C5-C6-O6	-5.55	125.27	128.60
1	A	1104	G	C8-N9-C4	-5.54	104.18	106.40
1	A	1206	G	N9-C4-C5	-5.53	103.19	105.40
1	A	1456	G	C8-N9-C1'	5.52	134.18	127.00
1	A	1290	G	N7-C8-N9	5.52	115.86	113.10
1	A	1382	C	C6-N1-C2	-5.52	118.09	120.30
1	A	343	U	C5-C6-N1	5.52	125.46	122.70
1	A	375	U	N3-C4-C5	-5.51	111.29	114.60
1	A	106	C	C6-N1-C2	-5.51	118.09	120.30
1	A	1395	C	C5-C6-N1	5.51	123.75	121.00
1	A	1030(C)	G	N7-C8-N9	5.51	115.86	113.10
1	A	1288	A	N1-C6-N6	-5.51	115.29	118.60
1	A	1025	U	N3-C2-O2	-5.50	118.35	122.20
1	A	203	U	C6-N1-C2	-5.50	117.70	121.00
1	A	968	A	C5-C6-N6	-5.50	119.30	123.70
1	A	1124	G	N3-C4-C5	-5.50	125.85	128.60
1	A	342	C	N1-C2-O2	-5.49	115.61	118.90
1	A	841	U	C5-C6-N1	5.49	125.44	122.70
1	A	1074	G	N1-C6-O6	5.49	123.19	119.90
1	A	1442	G	C5-C6-O6	5.49	131.89	128.60
1	A	1473	A	C8-N9-C4	5.49	107.99	105.80
1	A	436	C	N1-C2-N3	-5.48	115.37	119.20
1	A	402	G	N1-C2-N2	-5.47	111.28	116.20
1	A	1057	G	N9-C4-C5	-5.47	103.21	105.40
1	A	1204	A	C5-C6-N6	5.46	128.07	123.70
1	A	1148	U	C5-C6-N1	5.45	125.43	122.70
3	C	52	LEU	N-CA-C	5.45	125.72	111.00
1	A	361	G	C2-N3-C4	-5.45	109.18	111.90
1	A	1170	A	N1-C6-N6	-5.45	115.33	118.60
1	A	1366	C	N3-C4-C5	-5.44	119.72	121.90
1	A	771	G	N3-C4-C5	5.43	131.32	128.60
1	A	1502	A	C6-C5-N7	-5.43	128.50	132.30
1	A	784	C	C6-N1-C2	-5.43	118.13	120.30
1	A	278	G	C8-N9-C4	-5.43	104.23	106.40
1	A	361	G	N1-C2-N2	5.43	121.08	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	A	C4-C5-N7	-5.42	107.99	110.70
1	A	1125	U	N1-C2-O2	5.42	126.59	122.80
1	A	399	G	N1-C2-N3	-5.42	120.65	123.90
1	A	1220	G	C8-N9-C4	-5.41	104.23	106.40
1	A	1277	C	N1-C2-O2	5.41	122.14	118.90
1	A	44	G	N1-C2-N2	5.41	121.06	116.20
1	A	399	G	C6-N1-C2	5.40	128.34	125.10
1	A	266	G	C4-C5-N7	5.39	112.96	110.80
1	A	291	C	N3-C4-C5	-5.39	119.74	121.90
1	A	1094	G	C6-C5-N7	-5.39	127.17	130.40
1	A	1226	C	N1-C2-O2	-5.39	115.67	118.90
1	A	1081	G	C5-C6-O6	-5.38	125.37	128.60
1	A	894	G	C8-N9-C4	5.37	108.55	106.40
1	A	243	A	C8-N9-C4	-5.37	103.65	105.80
1	A	347	G	C2-N3-C4	-5.37	109.22	111.90
1	A	1118	C	C6-N1-C2	-5.37	118.15	120.30
1	A	1525	G	C5-C6-O6	5.36	131.82	128.60
1	A	187	C	C2-N1-C1'	5.36	124.70	118.80
1	A	353	A	C5-N7-C8	-5.36	101.22	103.90
1	A	1243	C	N1-C2-O2	-5.36	115.69	118.90
1	A	1473	A	N7-C8-N9	-5.36	111.12	113.80
1	A	204	U	C2-N1-C1'	5.35	124.12	117.70
1	A	266	G	N3-C4-N9	-5.35	122.79	126.00
1	A	300	A	C5-C6-N1	5.34	120.37	117.70
1	A	1030(A)	G	N7-C8-N9	5.34	115.77	113.10
1	A	403	C	N3-C4-N4	-5.34	114.26	118.00
1	A	361	G	N3-C2-N2	-5.34	116.16	119.90
1	A	1493	A	C8-N9-C4	-5.34	103.67	105.80
1	A	1026	G	N3-C4-C5	-5.33	125.94	128.60
1	A	1025	U	N1-C2-O2	5.33	126.53	122.80
1	A	870	U	C5-C4-O4	-5.32	122.71	125.90
1	A	621	A	N1-C6-N6	-5.32	115.41	118.60
1	A	890	G	C2-N3-C4	-5.32	109.24	111.90
1	A	925	G	N9-C4-C5	-5.32	103.27	105.40
1	A	1312	G	N9-C4-C5	5.32	107.53	105.40
1	A	1096	C	N1-C2-N3	5.31	122.92	119.20
1	A	749	C	C6-N1-C2	-5.31	118.18	120.30
1	A	560	U	C3'-C2'-C1'	5.30	105.74	101.50
1	A	560	U	C5-C6-N1	5.30	125.35	122.70
1	A	1058	G	N1-C6-O6	5.30	123.08	119.90
1	A	366	C	C2-N3-C4	-5.30	117.25	119.90
1	A	146	G	N3-C4-C5	-5.29	125.95	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1080	A	C5-C6-N1	-5.29	115.05	117.70
1	A	685	G	N1-C6-O6	5.29	123.07	119.90
1	A	896	C	C5-C6-N1	-5.29	118.36	121.00
1	A	1109	C	C5-C6-N1	-5.29	118.36	121.00
1	A	1039	C	N1-C2-O2	5.28	122.07	118.90
1	A	359	U	C2-N3-C4	-5.28	123.83	127.00
1	A	1459	C	O4'-C1'-N1	5.28	112.42	108.20
1	A	423	G	N3-C4-C5	-5.28	125.96	128.60
1	A	503	C	C2-N3-C4	5.27	122.54	119.90
1	A	1058	G	C5-C6-O6	-5.27	125.44	128.60
1	A	1057	G	N3-C4-N9	5.27	129.16	126.00
1	A	1029	C	C2-N1-C1'	5.27	124.60	118.80
1	A	1204	A	C5-C6-N1	-5.27	115.06	117.70
1	A	906	G	C6-C5-N7	-5.27	127.24	130.40
1	A	1504	G	C4-C5-C6	-5.27	115.64	118.80
1	A	915	A	N1-C6-N6	-5.27	115.44	118.60
1	A	355	C	C6-N1-C2	-5.26	118.19	120.30
1	A	54	C	C2-N3-C4	-5.26	117.27	119.90
1	A	768	A	C6-N1-C2	-5.26	115.44	118.60
1	A	1107	C	C6-N1-C2	-5.26	118.20	120.30
1	A	413	G	C6-C5-N7	5.25	133.55	130.40
1	A	880	C	N3-C4-N4	-5.25	114.32	118.00
1	A	1096	C	C2-N1-C1'	-5.25	113.02	118.80
1	A	1248	A	C8-N9-C4	-5.25	103.70	105.80
1	A	45	U	N1-C2-O2	-5.25	119.13	122.80
1	A	1089	G	N3-C2-N2	-5.24	116.23	119.90
1	A	1406	U	N3-C2-O2	-5.24	118.53	122.20
1	A	1037	C	C2-N1-C1'	5.24	124.56	118.80
1	A	1525	G	N1-C6-O6	-5.24	116.76	119.90
1	A	1081	G	N9-C4-C5	-5.23	103.31	105.40
1	A	1321	C	C5-C6-N1	5.22	123.61	121.00
1	A	631	G	C8-N9-C4	-5.22	104.31	106.40
1	A	1277	C	C5-C6-N1	5.22	123.61	121.00
1	A	967	C	C6-N1-C2	5.22	122.39	120.30
12	L	29	GLY	N-CA-C	-5.22	100.05	113.10
1	A	824	C	C5-C6-N1	-5.21	118.39	121.00
1	A	1009	G	N1-C6-O6	-5.21	116.77	119.90
1	A	760	G	N3-C4-C5	5.21	131.20	128.60
12	L	92	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	1002	G	N7-C8-N9	5.21	115.70	113.10
1	A	1320	C	C5-C6-N1	5.20	123.60	121.00
1	A	403	C	N1-C2-O2	5.20	122.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	G	N1-C6-O6	5.20	123.02	119.90
1	A	413	G	N9-C4-C5	5.20	107.48	105.40
1	A	299	G	C5-C6-N1	-5.19	108.90	111.50
1	A	1442	G	N1-C6-O6	-5.19	116.78	119.90
1	A	1249	C	N3-C4-C5	-5.19	119.82	121.90
1	A	915	A	C4-C5-N7	-5.17	108.11	110.70
1	A	1206	G	C8-N9-C1'	-5.17	120.27	127.00
1	A	935	A	C6-N1-C2	5.17	121.70	118.60
1	A	836	G	C6-C5-N7	-5.17	127.30	130.40
1	A	1258	G	C6-N1-C2	5.17	128.20	125.10
1	A	993	G	N3-C4-C5	-5.16	126.02	128.60
1	A	59	A	C5-C6-N6	-5.16	119.57	123.70
1	A	1302	U	C2-N1-C1'	-5.16	111.51	117.70
1	A	732	C	C2-N3-C4	-5.16	117.32	119.90
1	A	1321	C	N3-C4-C5	-5.16	119.84	121.90
1	A	1397	C	C6-N1-C1'	-5.15	114.61	120.80
1	A	1363	C	C6-N1-C1'	5.15	126.98	120.80
1	A	1056	U	C2-N1-C1'	5.15	123.88	117.70
1	A	1527	C	C2-N3-C4	-5.15	117.33	119.90
1	A	559	A	C8-N9-C4	-5.14	103.74	105.80
1	A	495	A	C5-C6-N6	5.14	127.81	123.70
1	A	1056	U	N1-C2-O2	5.14	126.40	122.80
1	A	1500	A	C5-N7-C8	-5.14	101.33	103.90
1	A	923	A	C4-C5-C6	5.14	119.57	117.00
1	A	1308	U	C5-C4-O4	5.14	128.98	125.90
1	A	898	G	C4-N9-C1'	-5.14	119.82	126.50
1	A	1148	U	N3-C4-O4	5.14	123.00	119.40
1	A	929	G	N9-C4-C5	5.13	107.45	105.40
1	A	1138	G	N3-C4-N9	5.13	129.08	126.00
1	A	892	A	C6-N1-C2	-5.12	115.53	118.60
1	A	1020	U	C2-N1-C1'	-5.12	111.56	117.70
1	A	820	U	N3-C2-O2	5.12	125.78	122.20
1	A	1067	A	C4-C5-C6	5.11	119.56	117.00
1	A	590	C	N1-C2-O2	5.11	121.97	118.90
1	A	117	G	N1-C6-O6	5.11	122.97	119.90
1	A	1026	G	N3-C4-N9	5.11	129.06	126.00
1	A	297	G	C5-C6-O6	-5.10	125.54	128.60
1	A	813	U	C5-C4-O4	-5.10	122.84	125.90
1	A	588	G	C8-N9-C4	5.09	108.44	106.40
1	A	154	C	C6-N1-C2	5.09	122.34	120.30
1	A	365	U	C4-C5-C6	5.09	122.76	119.70
1	A	42	G	C6-N1-C2	5.09	128.15	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1326	C	C6-N1-C2	5.09	122.33	120.30
1	A	1421	G	N1-C6-O6	-5.09	116.85	119.90
1	A	242	C	N1-C2-O2	-5.09	115.85	118.90
1	A	858	G	C8-N9-C4	-5.09	104.37	106.40
1	A	1399	C	C5-C4-N4	-5.09	116.64	120.20
1	A	600	C	C6-N1-C2	5.08	122.33	120.30
1	A	458	C	C2-N1-C1'	5.08	124.39	118.80
1	A	1429	C	N3-C4-C5	5.08	123.93	121.90
1	A	637	G	C8-N9-C4	5.08	108.43	106.40
1	A	1206	G	N3-C4-C5	-5.08	126.06	128.60
1	A	155	C	N1-C2-O2	5.08	121.95	118.90
1	A	1129	C	N3-C2-O2	-5.08	118.34	121.90
1	A	203	U	C5-C6-N1	5.07	125.24	122.70
1	A	47	C	C2-N3-C4	5.07	122.44	119.90
1	A	266	G	N7-C8-N9	5.07	115.64	113.10
1	A	1124	G	C8-N9-C4	-5.07	104.37	106.40
1	A	1510	U	C5-C6-N1	-5.07	120.17	122.70
1	A	243	A	N9-C4-C5	5.07	107.83	105.80
1	A	151	A	C8-N9-C4	-5.06	103.78	105.80
1	A	784	C	N3-C4-C5	-5.06	119.88	121.90
1	A	908	A	C8-N9-C4	5.06	107.82	105.80
1	A	1207	G	N3-C4-C5	5.06	131.13	128.60
1	A	1276	G	C4-C5-N7	-5.06	108.78	110.80
1	A	932	C	N3-C2-O2	-5.06	118.36	121.90
1	A	54	C	N3-C4-N4	-5.05	114.47	118.00
1	A	886	G	N1-C6-O6	5.05	122.93	119.90
1	A	56	U	N1-C2-N3	5.04	117.93	114.90
1	A	742	G	N1-C2-N2	5.04	120.74	116.20
1	A	768	A	N1-C2-N3	5.04	131.82	129.30
1	A	1212	U	N1-C2-O2	5.03	126.32	122.80
1	A	114	U	N3-C4-O4	-5.03	115.88	119.40
1	A	353	A	C8-N9-C4	-5.03	103.79	105.80
1	A	1100	C	N3-C4-N4	-5.02	114.49	118.00
1	A	1370	G	C5-C6-N1	-5.02	108.99	111.50
1	A	281	G	N7-C8-N9	5.01	115.61	113.10
1	A	985	C	C6-N1-C2	-5.01	118.30	120.30
1	A	1391	U	N1-C2-O2	5.01	126.31	122.80
1	A	824	C	N3-C2-O2	5.01	125.41	121.90
1	A	40	C	N1-C2-N3	5.00	122.70	119.20

There are no chirality outliers.

All (15) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
2	B	237	ALA	Peptide
3	C	100	ALA	Peptide
3	C	46	GLU	Peptide
3	C	78	GLY	Peptide
4	D	29	PRO	Peptide
9	I	38	GLN	Peptide
10	J	33	GLN	Peptide
10	J	90	LEU	Peptide
12	L	26	ALA	Peptide
12	L	87	GLY	Peptide
13	M	65	LYS	Peptide
14	N	13	THR	Peptide
14	N	14	PRO	Peptide
18	R	31	LEU	Peptide

## 5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32056	0	16179	896	0
2	B	1817	0	1785	78	0
3	C	1453	0	1320	78	0
4	D	1537	0	1430	89	0
5	E	1106	0	1132	39	0
6	F	776	0	733	19	0
7	G	1164	0	1106	47	0
8	H	1049	0	1037	33	0
9	I	849	0	735	56	0
10	J	657	0	547	38	0
11	K	828	0	822	23	0
12	L	905	0	916	29	0
13	M	784	0	730	40	0
14	N	474	0	485	35	0
15	O	724	0	749	28	0
16	P	661	0	653	47	0
17	Q	819	0	880	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	514	0	530	18	0
19	S	549	0	468	25	0
20	T	773	0	836	32	0
21	U	180	0	173	9	0
22	Y	739	0	740	38	0
23	A	208	0	0	0	0
23	E	1	0	0	0	0
23	Q	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	411	0	0	32	0
25	D	2	0	0	1	0
25	E	4	0	0	0	0
25	F	1	0	0	0	0
25	K	1	0	0	0	0
25	L	1	0	0	0	0
25	P	4	0	0	0	0
25	Q	3	0	0	0	0
25	R	1	0	0	1	0
25	T	2	0	0	0	0
25	U	1	0	0	1	0
All	All	51057	0	33986	1502	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 18.

All (1502) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1164:G:H1	1:A:1172:C:N4	1.45	1.15
1:A:427:U:OP1	4:D:13:ARG:NH2	1.82	1.11
1:A:538:G:H5''	12:L:114:LYS:HB2	1.43	0.97
1:A:574:A:OP2	25:A:1923:HOH:O	1.81	0.97
1:A:1502:A:H2	1:A:1505:G:H1	1.07	0.96
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.44	0.95
1:A:1164:G:H1	1:A:1172:C:H42	0.99	0.93
1:A:1244:C:H42	1:A:1293:G:H1	1.01	0.91
1:A:1164:G:N2	1:A:1172:C:N3	2.17	0.91
1:A:1128:C:O2'	1:A:1130:A:N7	2.05	0.90
1:A:1305:G:N2	1:A:1331:G:O2'	2.04	0.89
2:B:87:ARG:HE	2:B:233:SER:HB2	1.38	0.88
1:A:573:A:OP2	25:A:1923:HOH:O	1.90	0.88
1:A:975:A:H4'	1:A:976:G:H5''	1.56	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:33:GLN:NE2	10:J:33:GLN:O	2.08	0.86
18:R:32:ARG:HA	18:R:69:THR:HG21	1.54	0.86
1:A:1244:C:N4	1:A:1293:G:H1	1.73	0.86
5:E:100:VAL:O	5:E:107:ARG:NH2	2.10	0.84
1:A:1256:A:H61	1:A:1278:U:H1'	1.43	0.83
1:A:1366:C:O2'	10:J:60:ARG:NH1	2.11	0.83
1:A:1030:C:N4	1:A:1032:G:O6	2.12	0.83
1:A:426:G:OP1	4:D:38:TYR:OH	1.96	0.82
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.61	0.82
1:A:1159:U:O4'	1:A:1182:G:N2	2.12	0.82
4:D:106:TYR:HD2	4:D:107:ARG:HG2	1.45	0.82
9:I:18:PHE:HD1	9:I:62:TYR:HD2	1.26	0.81
1:A:1239:A:H2'	1:A:1298:C:H42	1.42	0.81
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.63	0.81
1:A:472:A:O2'	16:P:82:GLN:N	2.13	0.80
1:A:1053:G:N2	25:A:2249:HOH:O	2.14	0.80
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.64	0.79
1:A:652:U:OP2	25:A:1994:HOH:O	2.00	0.79
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.63	0.79
2:B:69:LEU:HB3	2:B:162:ILE:HG22	1.63	0.79
1:A:1164:G:N1	1:A:1172:C:N4	2.29	0.79
1:A:390:C:O3'	16:P:28:ARG:NH2	2.15	0.79
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.23	0.79
22:Y:23:ARG:NH1	22:Y:75:ASN:OD1	2.16	0.79
22:Y:87:LYS:O	22:Y:91:LYS:HB2	1.84	0.78
1:A:922:G:H4'	5:E:20:GLN:HA	1.65	0.78
1:A:1505:G:OP2	25:A:1944:HOH:O	2.02	0.78
1:A:1442:G:N7	1:A:1442(A):G:C6	2.51	0.78
1:A:1123:A:H4'	10:J:37:PRO:HG2	1.67	0.77
1:A:1499:A:OP2	25:A:1944:HOH:O	2.02	0.77
1:A:1459:C:H41	1:A:1461:G:N2	1.81	0.77
1:A:1151:A:H5'	10:J:41:PRO:HA	1.64	0.77
22:Y:53:THR:HG22	22:Y:62:VAL:HG12	1.64	0.77
1:A:1396:A:OP2	25:A:2086:HOH:O	2.02	0.77
1:A:1442:G:N7	1:A:1442(A):G:C5	2.53	0.77
10:J:48:THR:HA	10:J:62:HIS:HB3	1.65	0.77
1:A:950:U:H1'	1:A:971:G:N7	1.99	0.77
1:A:986:A:H1'	19:S:54:GLY:O	1.84	0.77
2:B:185:ILE:HG22	2:B:199:TYR:HB2	1.65	0.77
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.50	0.77
1:A:1441:G:H21	1:A:1459:C:H6	1.30	0.76
1:A:1065:U:H6	1:A:1190:G:H21	1.32	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1295:G:H21	1:A:1302:U:H3	1.34	0.76
6:F:11:ASN:HB3	6:F:14:LEU:HG	1.65	0.76
1:A:353:A:H5'	1:A:353:A:H8	1.49	0.76
1:A:1441:G:H4'	1:A:1442:G:N7	1.99	0.76
1:A:343:U:O2'	1:A:344:A:OP2	2.04	0.75
1:A:1026:G:H3'	1:A:1027:C:H5''	1.68	0.75
1:A:1502:A:H2	1:A:1505:G:N1	1.81	0.75
1:A:954:G:H21	1:A:1227:A:N6	1.85	0.75
1:A:581:G:N7	25:A:1960:HOH:O	2.20	0.75
1:A:1348:U:H4'	9:I:120:ARG:HG3	1.68	0.74
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.68	0.74
1:A:1459:C:C6	1:A:1460:A:N7	2.56	0.74
4:D:15:GLU:HG3	4:D:63:LYS:HG2	1.67	0.74
1:A:984:C:H2'	1:A:985:C:H6	1.53	0.74
2:B:21:ARG:H	2:B:21:ARG:HD2	1.52	0.73
1:A:642:A:N3	8:H:113:SER:OG	2.21	0.73
1:A:1456:G:O2'	20:T:39:LYS:NZ	2.21	0.73
1:A:425:G:H4'	4:D:45:GLN:HE22	1.53	0.73
1:A:673:G:H2'	1:A:674:G:C8	2.24	0.73
1:A:976:G:H5'	1:A:1358:U:O2'	1.89	0.73
2:B:15:VAL:HG23	2:B:209:ARG:HG2	1.68	0.72
9:I:21:PRO:HA	9:I:59:PHE:HA	1.71	0.72
1:A:1459:C:N3	1:A:1460:A:N6	2.37	0.72
10:J:54:PHE:HD2	10:J:55:LYS:HG3	1.54	0.72
13:M:4:ILE:HG21	13:M:9:ILE:HD12	1.70	0.72
1:A:921:U:O2	5:E:19:MET:HB2	1.88	0.72
1:A:192:U:O4'	20:T:102:GLY:HA2	1.90	0.72
2:B:201:ILE:HG21	2:B:214:ILE:HG21	1.72	0.72
1:A:222:U:H2'	1:A:223:U:C6	2.25	0.72
1:A:1348:U:H2'	1:A:1349:A:H8	1.54	0.71
1:A:992:U:O2'	1:A:993:G:OP2	2.04	0.71
1:A:1376:U:H2'	1:A:1377:A:C8	2.24	0.71
1:A:829:G:N7	25:A:1978:HOH:O	2.23	0.71
2:B:194:PRO:O	2:B:196:LEU:N	2.23	0.71
1:A:538:G:OP2	12:L:115:LYS:HB2	1.91	0.71
1:A:986:A:N3	19:S:52:TYR:OH	2.22	0.71
1:A:343:U:O2'	1:A:345:C:N4	2.23	0.71
1:A:1401:G:O6	22:Y:83:ARG:NH2	2.23	0.71
1:A:1154:G:H2'	1:A:1155:G:H8	1.55	0.71
1:A:1442(A):G:C8	1:A:1442(B):A:C2	2.78	0.71
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.56	0.70
1:A:1367:C:H5'	10:J:60:ARG:HH11	1.55	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:A:H2'	1:A:172:A:C8	2.26	0.70
1:A:266:G:O2'	1:A:267:C:OP2	2.08	0.70
1:A:1500:A:OP1	25:A:1946:HOH:O	2.09	0.70
1:A:735:C:H2'	1:A:736:C:H6	1.56	0.70
1:A:538:G:OP1	12:L:115:LYS:N	2.24	0.70
1:A:1004:A:H62	1:A:1037:C:H3'	1.56	0.70
1:A:750:G:N3	15:O:23:GLY:HA3	2.06	0.70
1:A:1442:G:O2'	1:A:1442(A):G:OP1	2.09	0.70
1:A:266:G:H5'	1:A:268:C:H41	1.57	0.69
9:I:40:LEU:HB3	9:I:43:ALA:HB2	1.73	0.69
1:A:437:U:H5''	4:D:155:LEU:HD11	1.73	0.69
1:A:446:G:N7	25:A:2157:HOH:O	2.25	0.69
1:A:595:G:O3'	25:A:1981:HOH:O	2.09	0.69
1:A:920:U:H2'	1:A:921:U:C6	2.27	0.69
1:A:472:A:HO2'	16:P:82:GLN:H	1.38	0.69
1:A:1220:G:O2'	19:S:52:TYR:O	2.11	0.69
9:I:4:TYR:HB2	9:I:19:LEU:HB2	1.75	0.69
6:F:82:ARG:HH11	6:F:82:ARG:HG3	1.57	0.69
1:A:1183:A:O2'	1:A:1184:G:OP1	2.11	0.69
1:A:860:A:OP2	25:A:1983:HOH:O	2.10	0.69
8:H:73:ASP:OD2	8:H:75:ARG:HD3	1.92	0.69
9:I:16:ARG:HB2	9:I:64:THR:HG23	1.74	0.69
1:A:1435:G:H2'	1:A:1436:U:C6	2.28	0.69
1:A:67:C:H2'	1:A:68:G:C8	2.27	0.69
1:A:1391:U:H2'	1:A:1392:G:C8	2.28	0.68
1:A:1349:A:H2'	1:A:1350:A:H8	1.58	0.68
1:A:408:A:OP1	4:D:113:SER:OG	2.11	0.68
1:A:1329:A:OP2	21:U:7:ARG:NH2	2.25	0.68
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.74	0.68
1:A:1378:C:H5	1:A:1379:G:C4	2.10	0.68
1:A:17:U:H2'	1:A:18:C:C6	2.29	0.68
1:A:1192:C:OP2	3:C:4:LYS:NZ	2.25	0.68
7:G:135:VAL:HA	7:G:138:LYS:HB3	1.74	0.68
1:A:1255:G:OP1	10:J:45:ARG:NH2	2.25	0.68
3:C:117:ALA:HB2	3:C:200:ALA:HB2	1.76	0.68
16:P:28:ARG:NH1	16:P:29:ASP:OD2	2.27	0.68
1:A:1169:A:H2'	1:A:1170:A:C8	2.28	0.68
1:A:664:G:H22	1:A:741:G:H1	1.40	0.68
1:A:1178:G:N2	1:A:1181:G:OP2	2.15	0.67
2:B:87:ARG:NE	2:B:233:SER:HB2	2.10	0.67
5:E:50:GLU:HB2	5:E:53:LEU:HD13	1.75	0.67
1:A:1226:C:N4	13:M:104:ARG:HD3	2.09	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1508:G:OP1	25:A:1946:HOH:O	2.11	0.67
2:B:91:PRO:HG2	2:B:155:LEU:HD23	1.76	0.67
1:A:610:G:O6	25:A:1939:HOH:O	2.08	0.67
1:A:1362:C:H2'	1:A:1363:C:H5''	1.76	0.67
13:M:69:GLU:HG3	13:M:70:LEU:H	1.60	0.67
2:B:116:GLU:HA	2:B:119:GLU:HB2	1.76	0.67
3:C:114:PRO:HA	3:C:185:GLY:HA3	1.76	0.67
11:K:86:GLY:N	11:K:112:THR:OG1	2.21	0.67
1:A:1004:A:N7	1:A:1037:C:H2'	2.09	0.67
16:P:28:ARG:HH11	16:P:28:ARG:HG2	1.58	0.67
14:N:21:TYR:OH	14:N:23:ARG:NH2	2.28	0.67
1:A:376:G:H5''	16:P:5:ARG:HD2	1.77	0.67
9:I:46:ALA:O	9:I:49:PRO:HD2	1.94	0.67
1:A:406:G:N3	4:D:119:GLN:NE2	2.43	0.66
1:A:344:A:H4'	1:A:345:C:OP2	1.93	0.66
1:A:436:C:H4'	4:D:156:GLU:HB2	1.77	0.66
1:A:412:A:O4'	4:D:35:ARG:NH2	2.27	0.66
1:A:1251:A:O2'	1:A:1369:C:O2'	2.09	0.66
2:B:163:PHE:CD2	2:B:185:ILE:HG13	2.31	0.66
7:G:150:ALA:HA	11:K:59:TYR:HB3	1.77	0.66
18:R:53:ARG:HH21	18:R:60:ALA:N	1.92	0.66
1:A:1347:G:C8	9:I:107:ARG:HB3	2.30	0.66
1:A:1459:C:H2'	1:A:1460:A:C8	2.30	0.66
1:A:976:G:H22	1:A:1363(A):A:H2'	1.59	0.66
1:A:1492:A:H5'	1:A:1493:A:C8	2.30	0.66
1:A:1441:G:H4'	1:A:1442:G:C8	2.30	0.66
1:A:1162:C:H42	1:A:1174:G:H1	1.44	0.65
13:M:65:LYS:HA	13:M:66:LEU:HB2	1.78	0.65
16:P:51:VAL:HG12	16:P:53:VAL:H	1.61	0.65
1:A:1442:G:O2'	1:A:1442(A):G:H5'	1.95	0.65
1:A:1154:G:H2'	1:A:1155:G:C8	2.31	0.65
3:C:35:GLU:HA	3:C:38:ARG:HD2	1.79	0.65
1:A:428:G:H5''	4:D:7:PRO:HB3	1.78	0.65
1:A:1412:C:H2'	1:A:1413:A:C8	2.31	0.65
1:A:990:C:N3	1:A:1215:G:O6	2.29	0.65
1:A:1059:C:OP1	3:C:199:LYS:NZ	2.27	0.65
1:A:165:C:H2'	1:A:166:G:C8	2.31	0.65
3:C:111:LEU:HD22	3:C:146:ALA:HB2	1.77	0.65
1:A:186:C:H2'	1:A:187:C:H6	1.61	0.65
1:A:457:C:H2'	1:A:458:C:H6	1.60	0.65
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.77	0.65
1:A:594:G:OP2	25:A:2300:HOH:O	2.13	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:584:G:H5'	17:Q:91:ARG:HH22	1.62	0.65
20:T:72:LEU:HD11	20:T:80:ARG:HD2	1.79	0.65
4:D:188:LEU:HD23	4:D:188:LEU:H	1.59	0.65
17:Q:22:LEU:HD13	17:Q:41:LYS:HG2	1.78	0.65
1:A:984:C:H2'	1:A:985:C:C6	2.30	0.65
1:A:1030(A):G:N2	1:A:1030(C):G:H3'	2.11	0.65
20:T:73:HIS:HB3	20:T:74:LYS:HG2	1.80	0.64
1:A:1309:G:N7	13:M:99:ARG:NH2	2.45	0.64
1:A:177:C:OP1	20:T:65:LYS:NZ	2.25	0.64
3:C:180:ALA:HA	3:C:206:GLU:HA	1.79	0.64
1:A:1181:G:H2'	1:A:1182:G:C5	2.33	0.64
1:A:1188:A:H2'	1:A:1189:C:O4'	1.98	0.64
1:A:1060:C:H5'	14:N:45:ARG:HH12	1.62	0.64
8:H:120:THR:H	8:H:123:GLU:HB2	1.62	0.64
1:A:179:A:N7	25:A:2206:HOH:O	2.30	0.64
5:E:143:ARG:NH1	8:H:77:GLU:OE1	2.30	0.64
1:A:954:G:H21	1:A:1227:A:H62	1.42	0.64
1:A:243:A:H4'	1:A:244:U:O5'	1.96	0.64
1:A:1318:A:H1'	19:S:37:ARG:HH21	1.61	0.64
1:A:426:G:OP1	4:D:36:ARG:NH1	2.31	0.64
2:B:21:ARG:N	2:B:21:ARG:HD2	2.11	0.63
1:A:1084:G:H5'	1:A:1102:A:OP2	1.97	0.63
5:E:80:ILE:HD12	5:E:138:ALA:HB1	1.80	0.63
1:A:1280:A:H5'	10:J:41:PRO:HD2	1.81	0.63
5:E:51:VAL:O	5:E:55:VAL:HG23	1.97	0.63
7:G:149:ARG:HD2	11:K:59:TYR:CE1	2.34	0.63
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.80	0.63
22:Y:30:TRP:HD1	22:Y:89:GLN:HG3	1.64	0.63
2:B:134:GLU:HA	2:B:137:ARG:HE	1.64	0.63
1:A:1170:A:N6	1:A:1171:G:N3	2.45	0.63
3:C:77:ILE:O	3:C:84:ILE:N	2.31	0.63
1:A:544:G:OP1	4:D:62:GLN:NE2	2.19	0.63
1:A:1170:A:C6	1:A:1171:G:H1'	2.33	0.63
1:A:1493:A:O2'	1:A:1494:G:OP1	2.15	0.63
1:A:402:G:O2'	1:A:620:C:N3	2.31	0.63
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.22	0.63
1:A:73:G:H1	1:A:96:U:H3	1.46	0.62
22:Y:54:ILE:HB	22:Y:61:LEU:HD12	1.81	0.62
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.14	0.62
3:C:100:ALA:O	3:C:102:ASN:N	2.30	0.62
1:A:838:G:H2'	1:A:839:U:H5''	1.80	0.62
1:A:542:G:P	4:D:10:ARG:HH22	2.22	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:43:LEU:O	20:T:47:GLY:N	2.31	0.62
20:T:30:LYS:HA	20:T:33:ILE:HD12	1.82	0.62
2:B:163:PHE:HA	2:B:185:ILE:HG12	1.81	0.62
1:A:612:C:O2	1:A:629:G:N2	2.32	0.62
3:C:92:ALA:HB2	3:C:99:VAL:H	1.63	0.62
1:A:1226:C:H4'	19:S:80:TYR:CZ	2.34	0.62
1:A:920:U:H2'	1:A:921:U:H6	1.64	0.62
1:A:1129:C:N4	1:A:1134:G:N7	2.48	0.62
1:A:769:G:H4'	1:A:1513:A:H4'	1.82	0.62
2:B:178:ARG:NH2	8:H:68:ARG:HH22	1.97	0.62
1:A:954:G:OP1	22:Y:17:ARG:NH2	2.33	0.62
21:U:5:ASP:O	21:U:11:GLY:HA3	1.99	0.62
1:A:222:U:H2'	1:A:223:U:H6	1.64	0.61
1:A:1089:G:H1	1:A:1096:C:H42	1.48	0.61
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.83	0.61
1:A:1316:G:N2	1:A:1319:A:O5'	2.32	0.61
1:A:430:A:OP1	4:D:9:CYS:N	2.34	0.61
2:B:236:TYR:CG	2:B:239:VAL:HB	2.35	0.61
1:A:405:U:O4	4:D:2:GLY:N	2.34	0.61
6:F:76:ALA:O	6:F:80:ARG:HG3	2.00	0.61
1:A:300:A:O2'	1:A:564:C:N3	2.29	0.61
7:G:20:ASP:HB3	7:G:23:VAL:HG23	1.81	0.61
4:D:13:ARG:NH1	4:D:38:TYR:O	2.32	0.61
9:I:71:SER:O	9:I:75:ASP:HB2	2.00	0.61
1:A:656:C:O2'	15:O:28:GLN:NE2	2.19	0.61
18:R:71:LYS:NZ	25:R:101:HOH:O	2.16	0.61
1:A:1161:C:H2'	1:A:1162:C:C6	2.35	0.61
1:A:1244:C:N3	1:A:1293:G:N2	2.40	0.61
1:A:827:U:H5''	1:A:828:A:OP2	2.00	0.61
1:A:437:U:H5''	4:D:155:LEU:HD21	1.82	0.61
1:A:1238:A:N3	1:A:1241:G:O2'	2.31	0.61
1:A:664:G:P	18:R:64:ARG:HH21	2.23	0.61
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.35	0.61
13:M:49:THR:O	13:M:51:ALA:N	2.34	0.61
1:A:1227:A:OP1	19:S:80:TYR:OH	2.13	0.60
13:M:48:LEU:O	13:M:52:GLU:HB2	2.00	0.60
8:H:87:SER:HA	8:H:93:VAL:HG23	1.82	0.60
1:A:1090:U:H2'	1:A:1091:U:C6	2.36	0.60
3:C:70:VAL:O	3:C:106:VAL:N	2.34	0.60
15:O:24:SER:OG	15:O:24:SER:O	2.19	0.60
1:A:1278:U:H5''	1:A:1279:A:O4'	2.01	0.60
1:A:538:G:H5''	12:L:114:LYS:CB	2.25	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:437:U:O3'	4:D:125:HIS:CE1	2.55	0.60
21:U:3:LYS:NZ	25:U:101:HOH:O	2.34	0.60
1:A:473:G:H2'	1:A:474:G:H8	1.66	0.60
1:A:791:G:N1	1:A:1498:U:OP1	2.30	0.60
1:A:1014:A:C2	1:A:1219:U:H1'	2.37	0.60
13:M:91:ARG:NH2	13:M:97:PRO:O	2.35	0.60
2:B:69:LEU:HD13	2:B:91:PRO:HB2	1.84	0.60
1:A:143:A:H2	1:A:220:G:H1	1.50	0.60
1:A:93:G:HO2'	1:A:96:U:H6	1.49	0.60
1:A:353:A:H5'	1:A:353:A:C8	2.35	0.60
1:A:542:G:OP1	4:D:10:ARG:NH1	2.35	0.60
1:A:564:C:OP1	25:A:1906:HOH:O	2.17	0.60
1:A:1172:C:H2'	1:A:1173:G:H8	1.67	0.59
1:A:1157:A:H61	1:A:1178:G:H21	1.47	0.59
4:D:65:ARG:HG2	4:D:75:PHE:CD1	2.37	0.59
11:K:79:SER:HA	11:K:104:GLN:HB2	1.84	0.59
1:A:1089:G:C6	1:A:1090:U:C4	2.90	0.59
3:C:52:LEU:HB3	3:C:70:VAL:HG13	1.84	0.59
1:A:609:A:N7	25:A:1940:HOH:O	2.32	0.59
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.67	0.59
1:A:991:U:C4	1:A:1212:U:H1'	2.37	0.59
1:A:149:A:HO2'	1:A:150:C:H6	1.47	0.59
1:A:957:U:H4'	19:S:79:THR:HG23	1.83	0.59
13:M:92:HIS:CE1	13:M:98:VAL:HG21	2.37	0.59
1:A:1136:U:H5''	1:A:1137:C:C4	2.38	0.59
7:G:111:ARG:HB2	7:G:119:ARG:HD2	1.84	0.59
3:C:11:ARG:HB3	3:C:15:THR:H	1.66	0.59
1:A:1208:C:H2'	1:A:1209:C:C6	2.38	0.59
9:I:99:LEU:HB3	9:I:101:PHE:CD1	2.37	0.59
1:A:1401:G:OP1	22:Y:80:LYS:HE2	2.02	0.59
16:P:75:ARG:O	16:P:78:GLY:N	2.27	0.59
1:A:47:C:H42	1:A:361:G:H1	1.50	0.59
22:Y:16:ILE:HB	22:Y:71:TYR:OH	2.03	0.59
1:A:1456:G:N2	20:T:51:GLU:OE1	2.33	0.59
6:F:15:ASP:OD2	6:F:17:SER:N	2.24	0.59
1:A:1172:C:H2'	1:A:1173:G:C8	2.37	0.59
1:A:1348:U:H2'	1:A:1349:A:C8	2.35	0.59
1:A:828:A:H2'	1:A:829:G:O4'	2.03	0.59
1:A:1259:C:N4	1:A:1260:C:O2	2.35	0.59
10:J:55:LYS:HE3	10:J:56:HIS:CE1	2.37	0.59
2:B:19:HIS:ND1	2:B:189:ASP:OD2	2.25	0.59
1:A:100:C:H2'	1:A:101:A:C8	2.37	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:20:VAL:HG21	16:P:32:TYR:CD1	2.38	0.59
1:A:59:A:H1'	1:A:354:G:N2	2.18	0.58
1:A:977:A:H2'	1:A:977:A:N3	2.16	0.58
2:B:87:ARG:HE	2:B:233:SER:CB	2.13	0.58
3:C:149:ALA:HA	3:C:201:TYR:O	2.03	0.58
1:A:791:G:N2	1:A:1497:G:O3'	2.34	0.58
1:A:1321:C:H4'	13:M:87:TYR:CE2	2.39	0.58
1:A:64:G:H4'	1:A:65:U:H3'	1.85	0.58
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.34	0.58
1:A:544:G:OP2	4:D:66:ARG:NH2	2.37	0.58
18:R:47:THR:HG23	18:R:49:LYS:HG3	1.84	0.58
1:A:537:G:OP1	12:L:113:ARG:NH2	2.37	0.58
1:A:1068:G:N2	1:A:1191:A:H1'	2.19	0.58
1:A:1067:A:O2'	1:A:1068:G:OP2	2.15	0.58
1:A:826:C:H2'	1:A:827:U:C6	2.37	0.58
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.85	0.58
1:A:1352:C:OP1	21:U:3:LYS:NZ	2.24	0.58
1:A:1258:G:H2'	1:A:1259:C:C6	2.38	0.58
3:C:122:GLU:HA	3:C:125:GLU:HG3	1.86	0.58
11:K:85:ARG:HE	11:K:111:ASP:HB3	1.69	0.58
1:A:1273:G:H5'	1:A:1274:G:OP2	2.04	0.58
4:D:158:ILE:O	4:D:162:LEU:N	2.36	0.58
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.37	0.58
15:O:5:LYS:O	15:O:9:GLN:HG2	2.03	0.58
1:A:1457:G:H2'	1:A:1458:G:C8	2.39	0.58
19:S:43:GLU:CD	19:S:43:GLU:H	2.05	0.58
2:B:87:ARG:HD2	2:B:219:VAL:HG11	1.86	0.58
21:U:14:TRP:CE3	21:U:15:ARG:HG3	2.39	0.58
3:C:123:GLN:O	3:C:128:PHE:HB2	2.03	0.57
1:A:316:G:OP2	1:A:351:G:O2'	2.22	0.57
1:A:1441:G:O2'	1:A:1459:C:N3	2.32	0.57
1:A:435:C:N4	1:A:436:C:H41	2.02	0.57
1:A:1011:G:H1	1:A:1018:C:H42	1.52	0.57
1:A:662:G:H2'	1:A:663:A:C8	2.40	0.57
19:S:49:ILE:O	19:S:60:VAL:N	2.31	0.57
1:A:763:G:H2'	1:A:764:C:H6	1.69	0.57
1:A:922:G:N3	1:A:1398:A:H2	2.02	0.57
1:A:1414:U:H3	1:A:1486:G:H1	1.52	0.57
21:U:18:TYR:CD2	21:U:22:ARG:HD2	2.39	0.57
1:A:1157:A:H4'	1:A:1158:C:O5'	2.05	0.57
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.85	0.57
1:A:342:C:H5'	20:T:4:LYS:HE2	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:32:VAL:HB	5:E:58:ALA:HB1	1.86	0.57
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.87	0.57
1:A:964:A:N3	1:A:969:A:O2'	2.36	0.57
1:A:1163:C:H2'	1:A:1164:G:H8	1.69	0.57
1:A:1157:A:H61	1:A:1178:G:N2	2.03	0.57
1:A:539:A:H2'	1:A:540:G:C8	2.39	0.57
1:A:437:U:O2'	4:D:125:HIS:HE1	1.87	0.57
9:I:110:GLU:HG2	9:I:119:ALA:HB1	1.87	0.57
1:A:559:A:OP1	5:E:126:ARG:NH2	2.37	0.57
2:B:77:ALA:HB1	2:B:165:VAL:HG11	1.87	0.57
1:A:1244:C:H2'	1:A:1245:A:H8	1.70	0.57
2:B:84:GLU:OE1	2:B:216:SER:HA	2.04	0.57
1:A:1095:U:H5'	1:A:1109:C:O2	2.04	0.57
1:A:859:A:H2'	1:A:860:A:O4'	2.05	0.57
1:A:404:U:C5'	4:D:122:ARG:HD3	2.35	0.57
1:A:748:C:H4'	1:A:749:C:O5'	2.05	0.57
1:A:1052:U:H2'	1:A:1055:A:OP1	2.04	0.56
3:C:29:TYR:O	3:C:29:TYR:HD2	1.87	0.56
1:A:826:C:H2'	1:A:827:U:H6	1.71	0.56
13:M:69:GLU:C	13:M:71:ARG:H	2.08	0.56
1:A:1457:G:H2'	1:A:1458:G:H8	1.70	0.56
9:I:45:ALA:HB1	9:I:47:LEU:H	1.70	0.56
2:B:18:GLY:HA3	2:B:41:ILE:HD13	1.86	0.56
3:C:150:LYS:HE3	3:C:152:ILE:HD11	1.85	0.56
1:A:342:C:N4	1:A:343:U:O4	2.39	0.56
1:A:663:A:O3'	18:R:64:ARG:NH2	2.37	0.56
5:E:147:ASP:OD2	5:E:147:ASP:N	2.38	0.56
4:D:153:ARG:NH1	4:D:180:GLY:O	2.28	0.56
1:A:1161:C:H2'	1:A:1162:C:H6	1.69	0.56
14:N:29:ARG:NH1	14:N:42:ILE:HD11	2.20	0.56
18:R:58:LEU:HD12	18:R:62:GLU:OE1	2.06	0.56
1:A:976:G:C8	1:A:1362:C:N4	2.74	0.56
1:A:1347:G:N2	1:A:1373:G:H2'	2.19	0.56
1:A:186:C:H2'	1:A:187:C:C6	2.40	0.56
4:D:110:PHE:H	4:D:110:PHE:HD1	1.51	0.56
9:I:33:PHE:O	9:I:37:PHE:HB2	2.06	0.56
1:A:1112:C:C2	3:C:178:LEU:HB2	2.41	0.56
1:A:1145:C:H4'	1:A:1146:A:H5'	1.88	0.56
1:A:403:C:P	4:D:137:SER:HG	2.27	0.56
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.87	0.56
1:A:1061:G:O2'	1:A:1062:U:OP1	2.23	0.56
2:B:12:GLU:O	2:B:16:HIS:ND1	2.39	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:833:U:H2'	1:A:834:C:H6	1.71	0.56
19:S:32:LYS:HB3	19:S:57:HIS:HD2	1.71	0.56
1:A:437:U:C5'	4:D:155:LEU:HD21	2.35	0.56
1:A:366:C:N3	25:A:2163:HOH:O	2.33	0.56
3:C:18:TRP:HE1	14:N:56:VAL:H	1.54	0.56
1:A:1292:U:H2'	1:A:1293:G:O4'	2.06	0.55
19:S:32:LYS:HB3	19:S:57:HIS:CD2	2.41	0.55
20:T:47:GLY:HA2	20:T:48:LYS:HB2	1.87	0.55
1:A:1184:G:H2'	1:A:1185:G:H8	1.71	0.55
1:A:1184:G:H2'	1:A:1185:G:C8	2.41	0.55
16:P:5:ARG:CZ	16:P:22:THR:HG21	2.35	0.55
3:C:153:VAL:HA	3:C:197:GLY:O	2.05	0.55
1:A:46:G:O2'	1:A:365:U:O2	2.24	0.55
1:A:131:C:H2'	1:A:132:C:H6	1.71	0.55
1:A:1255:G:O2'	1:A:1258:G:O2'	2.21	0.55
13:M:64:TRP:O	13:M:66:LEU:HG	2.06	0.55
1:A:1122:U:O4	1:A:1123:A:N6	2.38	0.55
1:A:1123:A:O2'	10:J:38:ILE:HG23	2.06	0.55
22:Y:30:TRP:CD1	22:Y:89:GLN:HG3	2.41	0.55
1:A:600:C:H2'	1:A:601:C:C6	2.40	0.55
1:A:935:A:H5''	25:A:2198:HOH:O	2.06	0.55
4:D:155:LEU:HD23	4:D:156:GLU:N	2.21	0.55
1:A:1330:U:H4'	13:M:23:TYR:CE2	2.41	0.55
1:A:1002:G:C2	1:A:1003:G:H1'	2.41	0.55
1:A:938:A:C6	1:A:939:G:C5	2.95	0.55
4:D:126:ILE:HG22	4:D:127:THR:H	1.70	0.55
4:D:100:ARG:HH12	4:D:137:SER:HB3	1.71	0.55
14:N:37:PHE:CE1	14:N:53:LEU:HD13	2.42	0.55
4:D:106:TYR:CD2	4:D:107:ARG:HG2	2.34	0.55
3:C:122:GLU:O	3:C:125:GLU:HB2	2.07	0.55
1:A:937:A:H1'	1:A:1379:G:H22	1.70	0.55
8:H:121:ASP:OD1	8:H:121:ASP:N	2.40	0.55
1:A:509:A:H5''	4:D:55:ALA:HB2	1.87	0.55
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.89	0.55
1:A:438:G:OP1	4:D:125:HIS:NE2	2.37	0.55
10:J:37:PRO:HA	10:J:72:VAL:HG12	1.89	0.55
1:A:1366:C:HO2'	10:J:60:ARG:HH12	1.51	0.55
7:G:135:VAL:O	7:G:139:GLU:N	2.25	0.55
22:Y:54:ILE:HB	22:Y:61:LEU:CD1	2.37	0.55
8:H:17:THR:HG22	8:H:63:LEU:HG	1.89	0.55
3:C:152:ILE:HB	3:C:199:LYS:HB2	1.87	0.54
1:A:1060:C:O2'	1:A:1061:G:H5'	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1016:A:H2'	1:A:1017:G:O4'	2.08	0.54
13:M:15:VAL:HG23	13:M:41:PRO:HA	1.88	0.54
12:L:49:ASN:ND2	12:L:92:ASP:OD2	2.41	0.54
1:A:520:A:O2'	12:L:73:GLU:OE1	2.17	0.54
1:A:1221:G:O3'	19:S:77:THR:OG1	2.24	0.54
1:A:1220:G:H1'	19:S:52:TYR:CD2	2.42	0.54
16:P:72:ARG:HG3	16:P:72:ARG:HH11	1.71	0.54
1:A:1360:A:H8	1:A:1360:A:OP1	1.89	0.54
1:A:57:G:H2'	1:A:58:C:C6	2.42	0.54
1:A:658:G:O4'	15:O:22:THR:HB	2.07	0.54
4:D:173:TRP:CD1	4:D:174:LEU:HG	2.42	0.54
7:G:92:SER:O	7:G:96:GLN:HG3	2.08	0.54
1:A:1067:A:O5'	1:A:1067:A:H8	1.90	0.54
9:I:17:VAL:HG21	9:I:80:GLY:C	2.27	0.54
11:K:19:ALA:HB3	11:K:82:VAL:HG22	1.88	0.54
21:U:18:TYR:HA	21:U:22:ARG:HB3	1.90	0.54
1:A:1151:A:O2'	1:A:1152:A:H8	1.90	0.54
1:A:1029:C:H42	1:A:1030:C:N4	2.05	0.54
1:A:1459:C:C5	1:A:1460:A:N7	2.76	0.54
1:A:171:A:H2'	1:A:172:A:H8	1.71	0.54
1:A:1342:C:H1'	9:I:124:GLN:HE21	1.72	0.54
1:A:1148:U:H2'	1:A:1149:C:O4'	2.06	0.54
15:O:17:ARG:HH11	15:O:17:ARG:CG	2.21	0.54
3:C:181:ASN:HB3	3:C:204:LEU:HB2	1.88	0.54
1:A:671:G:H2'	1:A:672:U:H6	1.72	0.54
1:A:950:U:H2'	1:A:951:G:H8	1.72	0.54
10:J:63:PHE:CD1	14:N:58:LYS:HA	2.43	0.54
1:A:407:G:H4'	4:D:116:GLN:HA	1.89	0.54
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.22	0.54
1:A:1095:U:OP1	1:A:1108:G:N2	2.38	0.54
1:A:192:U:H4'	20:T:57:ARG:HD2	1.90	0.54
1:A:952:U:H4'	1:A:964:A:N1	2.23	0.54
1:A:501:C:H2'	1:A:502:G:C8	2.43	0.54
5:E:145:LYS:O	5:E:149:GLU:HG2	2.08	0.54
1:A:1190:G:OP1	3:C:5:ILE:HB	2.08	0.54
1:A:1013:G:H2'	1:A:1015:A:OP2	2.08	0.54
9:I:59:PHE:HZ	9:I:88:TYR:CD1	2.26	0.54
2:B:187:LEU:HA	2:B:201:ILE:HB	1.90	0.54
22:Y:52:ALA:HB2	22:Y:77:LEU:HD11	1.89	0.54
2:B:87:ARG:HH21	2:B:233:SER:HB2	1.73	0.53
1:A:1123:A:C2	10:J:39:PRO:HD2	2.44	0.53
9:I:9:ARG:O	9:I:104:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:73:G:C6	1:A:97:G:C6	2.96	0.53
1:A:757:U:H2'	1:A:758:G:O4'	2.08	0.53
1:A:949:A:H61	1:A:1232:U:H3	1.55	0.53
1:A:427:U:OP2	4:D:36:ARG:NH2	2.36	0.53
1:A:1118:C:OP1	9:I:9:ARG:HD2	2.08	0.53
1:A:923:A:OP1	5:E:21:ALA:HB2	2.09	0.53
1:A:1030(A):G:N2	1:A:1031:G:C6	2.77	0.53
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.91	0.53
1:A:940:C:H2'	1:A:941:G:H8	1.73	0.53
2:B:236:TYR:HA	2:B:239:VAL:HG23	1.89	0.53
16:P:20:VAL:HG23	16:P:35:LYS:HA	1.90	0.53
9:I:14:VAL:O	9:I:65:VAL:HG23	2.08	0.53
1:A:1244:C:H2'	1:A:1245:A:C8	2.44	0.53
1:A:1106:G:H2'	1:A:1107:C:C6	2.44	0.53
2:B:194:PRO:C	2:B:196:LEU:H	2.11	0.53
1:A:1372:U:H2'	1:A:1373:G:O4'	2.08	0.53
1:A:56:U:H2'	1:A:57:G:C8	2.44	0.53
17:Q:76:LEU:HD11	17:Q:78:GLU:O	2.09	0.53
1:A:441:A:H3'	1:A:442:C:C6	2.43	0.53
1:A:141:A:H1'	1:A:182:U:O2	2.09	0.53
1:A:939:G:H2'	1:A:940:C:C6	2.43	0.53
1:A:1513:A:H2'	1:A:1514:C:C6	2.43	0.53
16:P:34:GLU:OE1	16:P:55:ARG:NH1	2.41	0.53
1:A:1198:G:H2'	1:A:1199:U:C6	2.44	0.53
7:G:57:GLU:HB3	7:G:60:LYS:H	1.72	0.53
2:B:178:ARG:HH21	8:H:74:PRO:HG3	1.73	0.53
3:C:48:TYR:O	3:C:51:GLY:N	2.41	0.53
2:B:17:PHE:HB3	2:B:44:LEU:HD11	1.90	0.53
7:G:38:LEU:O	7:G:42:ILE:HG13	2.09	0.53
1:A:1121:U:H2'	1:A:1122:U:H5'	1.91	0.53
1:A:991:U:C5	1:A:1212:U:H1'	2.44	0.53
11:K:85:ARG:HG2	11:K:112:THR:HA	1.91	0.53
1:A:1516:G:H2'	1:A:1518:A:OP2	2.09	0.53
19:S:22:LEU:HD13	19:S:28:LYS:H	1.74	0.53
1:A:768:A:OP2	25:A:2057:HOH:O	2.19	0.53
1:A:1122:U:H2'	1:A:1123:A:C8	2.44	0.53
1:A:1015:A:H1'	1:A:1219:U:H5'	1.90	0.53
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.90	0.53
1:A:1300:G:O2'	1:A:1301:U:OP2	2.24	0.53
1:A:1410:G:H2'	1:A:1411:C:C6	2.44	0.53
14:N:59:ALA:HB1	14:N:61:TRP:HZ3	1.74	0.53
5:E:102:ALA:O	5:E:107:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1297:C:O3'	7:G:114:ARG:NH2	2.40	0.52
14:N:29:ARG:HH21	14:N:41:ARG:HG2	1.74	0.52
2:B:236:TYR:HA	2:B:239:VAL:CG2	2.39	0.52
2:B:71:VAL:HG13	2:B:93:VAL:CG2	2.39	0.52
20:T:47:GLY:HA2	20:T:48:LYS:CB	2.40	0.52
13:M:90:LEU:C	13:M:92:HIS:H	2.12	0.52
1:A:814:A:N7	1:A:816:A:C4	2.77	0.52
9:I:18:PHE:HB2	9:I:62:TYR:HB3	1.91	0.52
1:A:1002:G:N3	1:A:1003:G:H1'	2.25	0.52
1:A:1118:C:H1'	1:A:1179:A:C4	2.45	0.52
2:B:82:ARG:HG3	2:B:92:TYR:OH	2.09	0.52
22:Y:40:ILE:HG13	22:Y:51:ASP:HB2	1.91	0.52
1:A:67:C:H2'	1:A:68:G:H8	1.74	0.52
7:G:120:ILE:O	7:G:124:LEU:HB2	2.10	0.52
1:A:450:G:H4'	16:P:41:PRO:HB2	1.91	0.52
4:D:129:ASN:HD21	4:D:144:ASP:HA	1.75	0.52
2:B:115:LEU:HD13	2:B:145:LEU:HB3	1.91	0.52
1:A:1021:G:H2'	1:A:1022:G:O4'	2.08	0.52
1:A:947:G:O3'	13:M:109:THR:OG1	2.25	0.52
1:A:1151:A:N3	10:J:39:PRO:HG3	2.24	0.52
1:A:393:A:OP2	16:P:12:LYS:HD2	2.10	0.52
1:A:1015:A:H2'	1:A:1016:A:C8	2.45	0.52
14:N:37:PHE:CZ	14:N:56:VAL:HG21	2.44	0.52
1:A:45:U:H2'	1:A:46:G:C8	2.45	0.52
16:P:68:ASP:O	16:P:71:ARG:HG2	2.10	0.52
21:U:10:ARG:HE	21:U:13:ILE:HD12	1.75	0.52
1:A:131:C:H2'	1:A:132:C:C6	2.45	0.52
1:A:1242:C:H2'	1:A:1243:C:O4'	2.10	0.52
1:A:1250:A:OP1	9:I:67:GLY:N	2.42	0.52
17:Q:18:THR:OG1	17:Q:69:LYS:NZ	2.30	0.52
1:A:448:A:P	1:A:485:G:H22	2.33	0.52
1:A:1277:C:HO2'	1:A:1279:A:H8	1.56	0.52
1:A:1442:G:C8	1:A:1442(A):G:C5	2.98	0.52
1:A:1286:A:H2'	1:A:1287:A:H4'	1.91	0.52
1:A:40:C:H42	1:A:402:G:H1	1.57	0.52
1:A:509:A:H3'	1:A:509:A:C8	2.44	0.52
8:H:13:ILE:O	8:H:17:THR:HG23	2.10	0.52
1:A:939:G:H1	1:A:1344:C:H42	1.57	0.52
7:G:134:ALA:O	7:G:138:LYS:N	2.34	0.52
7:G:151:TYR:OH	11:K:54:ARG:HG2	2.10	0.52
22:Y:12:ILE:HG22	22:Y:13:THR:H	1.75	0.52
22:Y:6:THR:O	22:Y:40:ILE:HA	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:413:G:H22	1:A:428:G:H1'	1.74	0.52
1:A:1206:G:C6	1:A:1207:G:C5	2.97	0.52
1:A:1321:C:H6	1:A:1322:C:H2'	1.74	0.52
4:D:31:CYS:C	4:D:33:MET:H	2.13	0.52
1:A:875:C:O2'	8:H:14:ARG:NH1	2.42	0.52
1:A:1066:C:H2'	1:A:1067:A:C8	2.44	0.51
1:A:1107:C:C4	1:A:1108:G:C8	2.97	0.51
1:A:1126:U:O2'	1:A:1127:G:O5'	2.23	0.51
1:A:376:G:H5''	16:P:5:ARG:HB2	1.90	0.51
1:A:413:G:N2	1:A:428:G:H1'	2.25	0.51
1:A:1335:C:H5'	1:A:1336:C:H5'	1.91	0.51
1:A:833:U:H2'	1:A:834:C:C6	2.45	0.51
14:N:60:SER:O	14:N:60:SER:OG	2.29	0.51
1:A:1349:A:C4	1:A:1350:A:C8	2.98	0.51
1:A:674:G:H2'	1:A:675:A:H8	1.75	0.51
10:J:55:LYS:HD2	10:J:56:HIS:H	1.76	0.51
6:F:82:ARG:NH1	6:F:82:ARG:HG3	2.20	0.51
1:A:412:A:N6	4:D:35:ARG:HA	2.25	0.51
4:D:188:LEU:CD2	4:D:188:LEU:H	2.23	0.51
4:D:10:ARG:HG3	4:D:11:LEU:HD12	1.91	0.51
15:O:8:LYS:HG2	15:O:12:ILE:HD11	1.91	0.51
7:G:51:GLN:O	7:G:55:GLY:HA2	2.10	0.51
13:M:43:THR:HB	13:M:47:ASP:HB2	1.92	0.51
1:A:1293:G:H2'	1:A:1294:G:C8	2.45	0.51
1:A:1288:A:N1	1:A:1371:G:H1'	2.24	0.51
1:A:994:A:N7	1:A:1216:G:H4'	2.25	0.51
22:Y:85:LEU:O	22:Y:89:GLN:HG2	2.10	0.51
16:P:72:ARG:HH21	16:P:73:LEU:HD21	1.75	0.51
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.90	0.51
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.44	0.51
18:R:31:LEU:O	18:R:32:ARG:HB2	2.11	0.51
4:D:59:ARG:O	4:D:63:LYS:HG3	2.10	0.51
1:A:1049:U:H4'	1:A:1050:G:C5'	2.40	0.51
1:A:438:G:P	4:D:125:HIS:HE2	2.34	0.51
11:K:86:GLY:H	11:K:112:THR:HG1	1.51	0.51
2:B:184:VAL:HG12	2:B:197:VAL:HG13	1.93	0.51
16:P:51:VAL:HG12	16:P:53:VAL:N	2.26	0.51
1:A:47:C:N4	1:A:361:G:H1	2.09	0.51
2:B:238:LEU:HB2	2:B:241:GLU:N	2.25	0.51
1:A:1004:A:H5''	1:A:1025:U:C4	2.46	0.51
1:A:1452:C:O2'	1:A:1456:G:OP2	2.27	0.51
1:A:149:A:O2'	1:A:150:C:P	2.69	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:434:U:H2'	1:A:435:C:C6	2.46	0.51
9:I:82:ALA:O	9:I:86:VAL:HG13	2.10	0.51
1:A:970:C:OP2	25:A:2045:HOH:O	2.20	0.51
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.50	0.51
1:A:940:C:H2'	1:A:941:G:C8	2.46	0.51
1:A:376:G:OP2	16:P:67:THR:HG21	2.10	0.51
20:T:10:LEU:HD23	20:T:12:ALA:H	1.76	0.51
9:I:27:THR:HG1	9:I:28:VAL:N	2.09	0.51
1:A:392:G:H2'	1:A:393:A:C8	2.46	0.51
1:A:1376:U:P	7:G:94:ARG:HH22	2.34	0.51
1:A:1343:G:C6	1:A:1344:C:C4	2.98	0.51
1:A:1326:C:H2'	1:A:1327:C:O4'	2.11	0.51
1:A:560:U:H4'	1:A:561:U:O5'	2.11	0.51
10:J:21:GLN:O	10:J:25:GLU:N	2.39	0.51
1:A:1386:G:C2	1:A:1387:G:C8	2.99	0.51
12:L:7:ILE:O	12:L:11:VAL:HG23	2.10	0.51
1:A:545:C:H5''	4:D:72:GLU:HG2	1.93	0.51
1:A:1300:G:O2'	1:A:1301:U:P	2.69	0.50
14:N:26:ARG:HD2	14:N:43:CYS:SG	2.50	0.50
1:A:1170:A:C5	1:A:1171:G:H1'	2.46	0.50
5:E:31:LEU:HD22	5:E:43:LEU:HD11	1.93	0.50
1:A:1122:U:N3	1:A:1123:A:C5	2.79	0.50
1:A:1028:C:H2'	1:A:1029:C:H6	1.76	0.50
1:A:1158:C:N3	1:A:1181:G:N2	2.58	0.50
1:A:1016:A:O5'	1:A:1016:A:H8	1.95	0.50
1:A:798:G:N7	25:A:2283:HOH:O	2.33	0.50
6:F:61:LEU:HB3	6:F:63:TYR:HE2	1.77	0.50
2:B:74:LYS:NZ	2:B:205:ASP:OD2	2.45	0.50
1:A:1281:U:H5''	1:A:1282:C:OP2	2.11	0.50
19:S:52:TYR:HB2	19:S:57:HIS:CE1	2.47	0.50
1:A:736:C:H2'	1:A:737:A:C8	2.46	0.50
1:A:937:A:C5	1:A:938:A:N7	2.79	0.50
1:A:101:A:O2'	1:A:102:G:H5'	2.11	0.50
1:A:1321:C:C6	1:A:1322:C:H2'	2.47	0.50
1:A:834:C:H2'	1:A:835:U:H6	1.77	0.50
1:A:196:A:OP1	20:T:68:LYS:NZ	2.36	0.50
1:A:544:G:P	4:D:62:GLN:HE21	2.32	0.50
1:A:1352:C:N4	1:A:1370:G:H1	2.08	0.50
1:A:1097:C:H2'	1:A:1098:C:C6	2.46	0.50
10:J:51:ARG:NE	10:J:61:GLU:HB2	2.27	0.50
16:P:6:LEU:HB3	16:P:17:TYR:CD2	2.47	0.50
1:A:270:A:H2'	1:A:271:C:C6	2.47	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:552:U:H4'	12:L:86:ARG:HG2	1.94	0.50
1:A:1030:C:H2'	1:A:1030(A):G:C8	2.45	0.50
1:A:1025:U:H1'	1:A:1026:G:N7	2.27	0.50
1:A:1376:U:H2'	1:A:1377:A:H8	1.76	0.50
1:A:1310:G:H5'	13:M:77:ASN:OD1	2.12	0.50
6:F:15:ASP:OD2	6:F:16:GLN:N	2.44	0.50
2:B:47:THR:O	2:B:51:LEU:N	2.35	0.50
1:A:373:A:H2'	1:A:374:A:H8	1.76	0.50
1:A:1068:G:N7	1:A:1094:G:C8	2.80	0.50
9:I:118:LYS:O	9:I:120:ARG:N	2.41	0.50
4:D:30:LYS:C	4:D:32:ALA:H	2.11	0.50
1:A:59:A:H1'	1:A:354:G:C2	2.47	0.50
8:H:33:GLU:HG3	8:H:59:LEU:HD11	1.93	0.50
1:A:1298:C:P	7:G:114:ARG:HH22	2.34	0.50
1:A:926:G:C6	22:Y:87:LYS:HG3	2.46	0.50
1:A:1206:G:H4'	3:C:192:THR:O	2.12	0.50
14:N:47:LEU:HA	14:N:50:LYS:HB2	1.93	0.50
1:A:262:A:H2'	1:A:263:A:C8	2.46	0.50
3:C:132:ARG:O	3:C:136:GLN:HB2	2.12	0.50
22:Y:24:LEU:HD22	22:Y:78:ILE:HD11	1.93	0.50
1:A:176:C:H2'	1:A:177:C:C6	2.47	0.50
2:B:162:ILE:HD11	2:B:184:VAL:HG22	1.93	0.50
1:A:392:G:H2'	1:A:393:A:H8	1.76	0.50
1:A:1095:U:P	1:A:1108:G:H1	2.33	0.50
1:A:1226:C:N4	13:M:104:ARG:HH11	2.09	0.50
7:G:113:GLU:CG	7:G:119:ARG:HG2	2.31	0.49
1:A:1030(A):G:N3	1:A:1030(C):G:C8	2.80	0.49
1:A:622:A:C8	1:A:623:C:C6	2.99	0.49
19:S:41:VAL:O	19:S:44:MET:HB2	2.12	0.49
22:Y:13:THR:O	22:Y:17:ARG:HG3	2.12	0.49
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.12	0.49
1:A:763:G:H2'	1:A:764:C:C6	2.47	0.49
1:A:618:C:N3	1:A:622:A:N6	2.60	0.49
13:M:6:GLY:HA3	13:M:22:ILE:HD13	1.93	0.49
1:A:1123:A:N3	10:J:38:ILE:HG22	2.27	0.49
14:N:4:LYS:HA	14:N:7:ILE:HG22	1.94	0.49
1:A:1386:G:N3	1:A:1387:G:C8	2.81	0.49
11:K:34:ASP:OD2	11:K:37:GLY:N	2.45	0.49
20:T:64:ASP:OD1	20:T:81:LYS:NZ	2.42	0.49
18:R:70:ILE:O	18:R:74:ARG:HG3	2.12	0.49
22:Y:70:MET:O	22:Y:74:ILE:HG12	2.12	0.49
22:Y:78:ILE:O	22:Y:82:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1063:C:OP2	1:A:1064:G:O2'	2.17	0.49
1:A:1064:G:OP1	1:A:1386:G:H4'	2.12	0.49
1:A:191:G:C6	1:A:192:U:N3	2.81	0.49
1:A:266:G:H5''	1:A:267:C:C5	2.48	0.49
1:A:600:C:C2	1:A:639:G:C2	3.00	0.49
10:J:35:SER:HB3	10:J:73:ASP:O	2.12	0.49
11:K:99:GLN:HG2	11:K:105:VAL:HG21	1.94	0.49
6:F:75:LEU:O	6:F:79:LEU:HG	2.13	0.49
1:A:403:C:OP1	4:D:137:SER:OG	2.18	0.49
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.48	0.49
11:K:44:SER:OG	11:K:47:VAL:HG23	2.12	0.49
17:Q:53:LEU:HD23	17:Q:82:MET:HE1	1.94	0.49
11:K:48:ILE:O	11:K:50:TYR:N	2.45	0.49
6:F:69:GLU:O	6:F:72:VAL:HG13	2.13	0.49
14:N:24:CYS:HB3	14:N:27:CYS:O	2.13	0.49
1:A:1106:G:H2'	1:A:1107:C:H6	1.76	0.49
1:A:1003:G:H2'	1:A:1004:A:C4'	2.42	0.49
1:A:1004:A:H5''	1:A:1025:U:O4	2.12	0.49
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.94	0.49
1:A:719:C:C2	18:R:50:ILE:HG12	2.48	0.49
1:A:1267:C:H2'	1:A:1267:C:O2	2.12	0.49
2:B:114:ARG:HD3	2:B:118:LEU:HG	1.93	0.49
3:C:138:VAL:HG23	3:C:151:VAL:HG23	1.93	0.49
1:A:974:A:P	14:N:41:ARG:HH12	2.34	0.49
2:B:53:ARG:HH12	2:B:199:TYR:HA	1.77	0.49
1:A:1295:G:N2	1:A:1302:U:H3	2.07	0.49
1:A:953:G:H4'	22:Y:6:THR:OG1	2.12	0.49
22:Y:13:THR:H	22:Y:16:ILE:HG23	1.77	0.49
4:D:15:GLU:OE2	4:D:66:ARG:NH1	2.46	0.49
1:A:302:G:N3	1:A:556:C:H4'	2.27	0.49
1:A:189(F):U:C4	17:Q:72:ARG:CZ	2.96	0.49
22:Y:12:ILE:HG22	22:Y:16:ILE:HG23	1.94	0.49
1:A:1493:A:HO2'	1:A:1494:G:P	2.35	0.49
18:R:45:SER:OG	18:R:47:THR:HG22	2.13	0.49
1:A:453:A:H4'	16:P:72:ARG:HG2	1.94	0.49
5:E:12:LEU:HB3	5:E:31:LEU:HB2	1.93	0.49
1:A:1306:A:H2'	1:A:1307:U:O4'	2.12	0.49
5:E:91:LEU:HD12	5:E:120:THR:HG22	1.95	0.49
2:B:68:ILE:HG12	2:B:161:ALA:HB3	1.94	0.49
1:A:404:U:H5'	4:D:122:ARG:HD3	1.95	0.49
13:M:49:THR:O	13:M:52:GLU:N	2.46	0.49
7:G:51:GLN:HG3	7:G:56:GLN:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:135:GLN:O	2:B:138:LEU:N	2.44	0.49
17:Q:95:TYR:O	17:Q:98:LEU:HB2	2.12	0.49
1:A:685:G:O2'	1:A:686:U:H5'	2.13	0.49
8:H:44:PHE:HE2	8:H:109:ILE:HD12	1.77	0.49
1:A:1381:U:H2'	1:A:1381:U:O2	2.13	0.49
1:A:1162:C:N4	1:A:1174:G:H1	2.09	0.49
1:A:165:C:H2'	1:A:166:G:H8	1.77	0.49
6:F:8:ILE:HD12	6:F:26:ILE:HD13	1.93	0.49
1:A:1316:G:H2'	1:A:1318:A:OP2	2.13	0.48
4:D:126:ILE:HG22	4:D:127:THR:N	2.27	0.48
8:H:33:GLU:HG2	8:H:48:TYR:CE1	2.48	0.48
1:A:530:G:H3'	1:A:531:U:C5'	2.43	0.48
1:A:674:G:H2'	1:A:675:A:C8	2.48	0.48
13:M:65:LYS:NZ	13:M:69:GLU:HG2	2.29	0.48
1:A:69:G:N3	1:A:70:G:C8	2.81	0.48
10:J:33:GLN:HE21	10:J:33:GLN:C	2.11	0.48
1:A:1508:G:H2'	1:A:1509:C:O4'	2.13	0.48
5:E:144:THR:OG1	5:E:147:ASP:OD2	2.19	0.48
1:A:616:G:C2	1:A:617:G:C8	3.00	0.48
7:G:44:TYR:HA	7:G:47:CYS:HB2	1.96	0.48
22:Y:69:ASP:HB3	22:Y:72:THR:HB	1.95	0.48
1:A:426:G:P	4:D:36:ARG:NH1	2.86	0.48
1:A:1358:U:H2'	1:A:1359:C:O4'	2.13	0.48
1:A:735:C:H2'	1:A:736:C:C6	2.42	0.48
1:A:1169:A:H2'	1:A:1170:A:H8	1.76	0.48
1:A:1446:U:H4'	1:A:1447:A:C5	2.48	0.48
1:A:1293:G:H2'	1:A:1294:G:H8	1.77	0.48
1:A:1064:G:O2'	1:A:1065:U:OP2	2.31	0.48
1:A:1060:C:C5	3:C:2:GLY:HA3	2.48	0.48
22:Y:12:ILE:HG22	22:Y:13:THR:N	2.27	0.48
1:A:148:G:O2'	1:A:149:A:H5'	2.14	0.48
1:A:1112:C:H1'	3:C:179:ARG:HG2	1.95	0.48
10:J:51:ARG:CZ	10:J:61:GLU:HB2	2.43	0.48
1:A:601:C:H2'	1:A:602:A:C8	2.49	0.48
3:C:25:GLY:O	3:C:27:LYS:N	2.45	0.48
1:A:731:G:H5'	1:A:766:A:H4'	1.94	0.48
1:A:1163:C:C2	1:A:1174:G:C2	3.02	0.48
1:A:1150:U:O4	1:A:1151:A:N6	2.46	0.48
2:B:54:THR:HG23	2:B:199:TYR:HB3	1.94	0.48
1:A:939:G:H1	1:A:1344:C:N4	2.11	0.48
1:A:1087:G:C6	1:A:1088:G:O6	2.66	0.48
1:A:429:U:H5'	4:D:9:CYS:HB2	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:51:VAL:CG1	16:P:53:VAL:H	2.24	0.48
1:A:9:G:H2'	1:A:10:A:H8	1.78	0.48
8:H:83:ILE:HB	8:H:137:VAL:HG13	1.95	0.48
1:A:684:A:H2'	1:A:685:G:C8	2.49	0.48
3:C:9:GLY:HA2	3:C:12:LEU:HG	1.96	0.48
1:A:1144:G:N2	1:A:1146:A:H62	2.12	0.48
12:L:34:ARG:O	12:L:61:THR:HG23	2.13	0.48
17:Q:84:LEU:O	17:Q:87:LYS:HB2	2.14	0.48
1:A:1043:C:H2'	1:A:1044:A:O4'	2.13	0.48
1:A:976:G:P	14:N:32:SER:H	2.37	0.48
9:I:104:ARG:NH1	9:I:105:ASP:O	2.43	0.48
1:A:149:A:O2'	1:A:150:C:H6	1.97	0.48
15:O:21:ASP:OD2	15:O:24:SER:HB3	2.14	0.48
1:A:57:G:H2'	1:A:58:C:H6	1.78	0.48
1:A:659:U:H2'	1:A:660:G:O4'	2.13	0.48
14:N:59:ALA:HB1	14:N:61:TRP:CZ3	2.49	0.48
1:A:1443:G:O6	1:A:1459:C:O2	2.32	0.48
1:A:425:G:H4'	4:D:45:GLN:NE2	2.27	0.48
1:A:1207:G:H2'	1:A:1208:C:C6	2.48	0.48
1:A:1235:U:O2'	1:A:1305:G:O5'	2.32	0.48
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.49	0.48
1:A:393:A:OP1	16:P:13:HIS:HE1	1.97	0.48
1:A:436:C:O2'	1:A:437:U:OP2	2.28	0.48
1:A:438:G:H5'	4:D:123:HIS:HB3	1.96	0.48
1:A:938:A:N6	1:A:939:G:C6	2.82	0.48
3:C:111:LEU:CD2	3:C:146:ALA:HB2	2.44	0.48
1:A:269:C:H2'	1:A:270:A:C8	2.49	0.48
8:H:29:SER:HB3	8:H:32:LYS:HG3	1.96	0.48
1:A:959:A:O2'	1:A:961:U:H5'	2.14	0.48
1:A:1323:G:H4'	1:A:1363:C:C2	2.49	0.47
1:A:1486:G:H2'	1:A:1487:G:O4'	2.14	0.47
4:D:120:LEU:HB3	4:D:126:ILE:HD11	1.96	0.47
1:A:942:G:C2	1:A:1342:C:C2	3.02	0.47
1:A:767:A:H2'	1:A:768:A:O4'	2.14	0.47
1:A:545:C:H5''	4:D:72:GLU:CB	2.44	0.47
1:A:1306:A:H2'	1:A:1307:U:C6	2.49	0.47
7:G:15:ASP:CB	7:G:19:GLY:H	2.27	0.47
1:A:930:C:C2'	1:A:931:C:H5'	2.44	0.47
1:A:1441:G:N3	1:A:1459:C:C5	2.82	0.47
2:B:54:THR:O	2:B:58:ILE:HG13	2.14	0.47
2:B:210:SER:O	2:B:214:ILE:HG12	2.14	0.47
1:A:254:G:OP1	17:Q:67:LYS:O	2.32	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:18:C:H4'	1:A:1078:U:O2	2.14	0.47
1:A:1321:C:C3'	1:A:1322:C:H5''	2.44	0.47
14:N:37:PHE:HZ	14:N:56:VAL:HG21	1.78	0.47
4:D:18:LYS:NZ	4:D:31:CYS:HB3	2.29	0.47
2:B:55:PHE:O	2:B:59:GLU:N	2.38	0.47
1:A:512:U:O2'	4:D:42:GLN:NE2	2.44	0.47
2:B:52:GLU:O	2:B:56:ARG:HG2	2.13	0.47
1:A:110:C:H2'	1:A:111:G:O4'	2.14	0.47
1:A:1004:A:H5''	1:A:1025:U:C5	2.49	0.47
16:P:5:ARG:HH11	16:P:5:ARG:HG3	1.79	0.47
1:A:542:G:H2'	1:A:543:C:H6	1.79	0.47
1:A:1330:U:H4'	13:M:23:TYR:HE2	1.77	0.47
1:A:947:G:H2'	1:A:948:C:O4'	2.14	0.47
5:E:36:ASP:OD2	5:E:38:GLN:N	2.41	0.47
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.49	0.47
3:C:130:VAL:HG12	3:C:134:ILE:HD11	1.96	0.47
1:A:1297:C:H4'	1:A:1298:C:H5'	1.97	0.47
1:A:974:A:OP2	14:N:41:ARG:NH1	2.47	0.47
1:A:664:G:N2	1:A:741:G:H1	2.07	0.47
5:E:89:ILE:HD13	5:E:90:VAL:H	1.78	0.47
1:A:516:U:C4	1:A:517:G:C6	3.02	0.47
1:A:174:C:H2'	1:A:175:C:H6	1.79	0.47
1:A:1292:U:H5'	9:I:38:GLN:HE21	1.79	0.47
1:A:413:G:N7	4:D:35:ARG:NH2	2.62	0.47
12:L:71:PRO:O	12:L:102:ARG:NH1	2.47	0.47
1:A:1225:A:N3	1:A:1225:A:H2'	2.29	0.47
6:F:36:ARG:HH11	6:F:36:ARG:CB	2.27	0.47
9:I:18:PHE:CD1	9:I:62:TYR:HD2	2.17	0.47
1:A:1060:C:H2'	1:A:1061:G:H8	1.79	0.47
1:A:750:G:H1'	15:O:23:GLY:H	1.79	0.47
1:A:97:G:O2'	1:A:98:G:H8	1.97	0.47
12:L:84:LEU:HD22	12:L:85:ILE:H	1.80	0.47
1:A:1442:G:HO2'	1:A:1442(A):G:P	2.30	0.47
9:I:19:LEU:HB3	9:I:59:PHE:CD1	2.50	0.47
1:A:1119:C:N3	1:A:1154:G:O6	2.47	0.47
18:R:53:ARG:HH21	18:R:60:ALA:H	1.62	0.47
1:A:990:C:C2	1:A:1216:G:C2	3.03	0.47
1:A:977:A:C2	1:A:1224:G:N7	2.82	0.47
1:A:834:C:H2'	1:A:835:U:C6	2.49	0.47
1:A:518:C:O2'	1:A:530:G:N2	2.48	0.47
3:C:12:LEU:HA	3:C:16:ARG:O	2.15	0.47
7:G:99:LEU:HD22	7:G:103:TRP:CZ2	2.49	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:127:ILE:C	2:B:129:GLU:H	2.18	0.47
1:A:604:G:C2	1:A:635:G:C5	3.03	0.47
1:A:631:G:H2'	1:A:632:A:C8	2.50	0.47
1:A:360:A:N1	25:A:1928:HOH:O	2.35	0.47
15:O:57:LEU:HA	15:O:57:LEU:HD23	1.75	0.47
3:C:186:PHE:HA	3:C:198:VAL:O	2.15	0.47
1:A:1006:C:H2'	1:A:1007:C:O4'	2.15	0.47
1:A:857:C:H2'	1:A:858:G:O4'	2.15	0.47
1:A:449:C:O2	16:P:42:ARG:HD2	2.15	0.47
3:C:130:VAL:O	3:C:132:ARG:N	2.42	0.47
4:D:30:LYS:CB	4:D:35:ARG:HD2	2.45	0.47
20:T:33:ILE:O	20:T:37:SER:OG	2.26	0.47
1:A:321:A:C2	1:A:333:G:C2	3.03	0.47
1:A:387:U:OP1	25:A:1903:HOH:O	2.20	0.47
10:J:32:ALA:O	10:J:76:ASN:N	2.44	0.47
1:A:199:G:O2'	1:A:200:G:H5'	2.15	0.47
1:A:1277:C:H2'	1:A:1278:U:H5'	1.97	0.47
1:A:937:A:H1'	1:A:1379:G:N2	2.30	0.47
1:A:1412:C:H2'	1:A:1413:A:H8	1.78	0.47
7:G:24:THR:O	7:G:27:ILE:HG12	2.15	0.47
1:A:1310:G:H1	1:A:1327:C:H42	1.62	0.47
1:A:620:C:H2'	1:A:621:A:O4'	2.15	0.47
10:J:12:ASP:HB3	10:J:15:THR:HG23	1.97	0.47
1:A:971:G:N1	1:A:1363(A):A:OP2	2.38	0.47
1:A:1028:C:H2'	1:A:1029:C:C6	2.50	0.47
9:I:27:THR:O	9:I:63:ILE:HB	2.15	0.47
1:A:966:G:C4	22:Y:62:VAL:HG11	2.50	0.47
1:A:433:C:O2'	1:A:434:U:H5'	2.15	0.47
15:O:56:LEU:O	15:O:60:VAL:HG23	2.15	0.47
9:I:83:ARG:O	9:I:86:VAL:HG22	2.16	0.47
1:A:868:C:H2'	1:A:869:G:O4'	2.15	0.47
1:A:129(A):G:C5	1:A:189(H):G:H1'	2.50	0.47
5:E:127:ASN:HA	5:E:128:PRO:HD3	1.80	0.47
1:A:1443:G:O6	1:A:1459:C:C2	2.68	0.46
2:B:53:ARG:NH2	2:B:198:ASP:O	2.39	0.46
10:J:54:PHE:CD2	10:J:55:LYS:HG3	2.43	0.46
20:T:73:HIS:HB3	20:T:74:LYS:HE2	1.96	0.46
1:A:561:U:HO2'	1:A:562:C:P	2.37	0.46
9:I:44:VAL:HA	9:I:45:ALA:HA	1.48	0.46
1:A:717:C:H6	1:A:717:C:H5''	1.79	0.46
7:G:111:ARG:HB3	7:G:113:GLU:OE1	2.15	0.46
1:A:973:G:C6	1:A:974:A:N6	2.83	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1227:A:H3'	1:A:1227:A:C8	2.50	0.46
8:H:19:VAL:HG23	8:H:21:LYS:HD3	1.98	0.46
20:T:5:LYS:HA	20:T:6:PRO:HD2	1.66	0.46
14:N:29:ARG:HH12	14:N:42:ILE:HD11	1.80	0.46
20:T:67:ALA:HA	20:T:72:LEU:O	2.15	0.46
15:O:26:GLU:HG2	15:O:26:GLU:H	1.26	0.46
1:A:9:G:H2'	1:A:10:A:C8	2.51	0.46
2:B:120:ALA:C	2:B:122:PHE:H	2.18	0.46
10:J:9:ARG:HA	10:J:16:LEU:HD11	1.97	0.46
3:C:164:ARG:HG2	3:C:165:THR:H	1.80	0.46
1:A:224:C:H2'	1:A:225:C:C6	2.50	0.46
1:A:1096:C:C4	1:A:1097:C:C5	3.04	0.46
13:M:69:GLU:C	13:M:71:ARG:N	2.69	0.46
1:A:601:C:H2'	1:A:602:A:H8	1.79	0.46
2:B:82:ARG:HG3	2:B:92:TYR:CZ	2.50	0.46
2:B:47:THR:HA	2:B:202:PRO:HG2	1.96	0.46
1:A:1333:A:H3'	1:A:1334:G:H8	1.81	0.46
1:A:1465:C:H2'	1:A:1466:C:O4'	2.14	0.46
5:E:81:GLU:HB3	5:E:88:LYS:HE2	1.98	0.46
1:A:750:G:C2	15:O:23:GLY:HA3	2.49	0.46
1:A:179:A:H2'	1:A:180:U:H6	1.80	0.46
1:A:1263:C:O2'	1:A:1264:C:H5'	2.16	0.46
1:A:1055:A:C2	1:A:1056:U:H1'	2.50	0.46
8:H:20:TYR:HD1	8:H:65:TYR:CD2	2.34	0.46
2:B:186:ALA:O	2:B:201:ILE:N	2.44	0.46
1:A:1087:G:N1	1:A:1088:G:C6	2.84	0.46
1:A:1215:G:C6	1:A:1216:G:C5	3.04	0.46
1:A:1316:G:N2	1:A:1318:A:H3'	2.30	0.46
1:A:300:A:H1'	1:A:565:U:O2	2.15	0.46
1:A:944:G:N1	1:A:1338:G:OP2	2.42	0.46
1:A:36:C:OP1	12:L:123:LYS:NZ	2.44	0.46
10:J:95:GLU:HG3	10:J:96:ILE:H	1.80	0.46
1:A:116:A:C8	1:A:116:A:OP2	2.69	0.46
22:Y:5:ILE:HG21	22:Y:20:VAL:HG11	1.97	0.46
1:A:983:A:H2	1:A:984:C:C6	2.34	0.46
1:A:438:G:H4'	4:D:123:HIS:ND1	2.30	0.46
1:A:1342:C:O2'	9:I:124:GLN:HG3	2.15	0.46
1:A:757:U:OP1	1:A:822:C:O2'	2.28	0.46
1:A:503:C:OP2	12:L:116:SER:HB3	2.15	0.46
2:B:27:LYS:HD2	2:B:193:ASP:OD1	2.15	0.46
1:A:1065:U:H4'	1:A:1066:C:O5'	2.15	0.46
1:A:1386:G:H2'	1:A:1387:G:H8	1.81	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:43:LEU:CD1	20:T:51:GLU:HG2	2.46	0.46
1:A:1102:A:H8	1:A:1102:A:H5''	1.79	0.46
1:A:838:G:C2'	1:A:839:U:H5''	2.46	0.46
13:M:15:VAL:O	13:M:19:LEU:HD23	2.15	0.46
1:A:942:G:H21	9:I:124:GLN:NE2	2.13	0.46
1:A:1009:G:C2	1:A:1010:G:C8	3.04	0.46
22:Y:67:HIS:HB3	22:Y:73:ALA:HB2	1.97	0.46
1:A:1323:G:H4'	1:A:1363:C:N3	2.30	0.46
1:A:1227:A:H3'	1:A:1227:A:H8	1.80	0.46
1:A:1084:G:C5	1:A:1085:U:C4	3.04	0.46
1:A:671:G:H2'	1:A:672:U:C6	2.51	0.46
1:A:624:C:H2'	1:A:625:G:H8	1.81	0.46
1:A:1000:U:C2'	1:A:1001:A:H5'	2.46	0.46
10:J:8:LEU:HG	10:J:8:LEU:H	1.59	0.46
1:A:1271:G:H5'	1:A:1314:C:H5''	1.97	0.46
1:A:1357:A:N7	1:A:1358:U:C5	2.84	0.46
5:E:104:ALA:O	5:E:107:ARG:HB3	2.16	0.46
1:A:343:U:H2'	1:A:343:U:H6	1.49	0.46
1:A:1349:A:H2'	1:A:1350:A:C8	2.43	0.46
1:A:750:G:H21	15:O:23:GLY:HA3	1.79	0.46
1:A:474:G:H2'	1:A:475:G:H8	1.81	0.46
1:A:177:C:P	20:T:65:LYS:NZ	2.89	0.46
1:A:1496:C:H2'	1:A:1497:G:O4'	2.16	0.46
3:C:65:ALA:HA	3:C:100:ALA:HB3	1.98	0.46
1:A:263:A:OP2	20:T:79:ARG:NH1	2.49	0.46
1:A:1438:G:H2'	1:A:1439:C:C6	2.51	0.46
5:E:8:GLU:HA	5:E:33:VAL:O	2.15	0.46
1:A:688:G:H2'	1:A:689:C:H6	1.80	0.46
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.98	0.46
1:A:114:U:H2'	1:A:115:G:C8	2.51	0.46
1:A:1366:C:H2'	1:A:1367:C:C6	2.50	0.45
9:I:26:VAL:HG22	9:I:61:ALA:N	2.30	0.45
1:A:1208:C:H2'	1:A:1209:C:H6	1.80	0.45
6:F:61:LEU:HB3	6:F:63:TYR:CE2	2.51	0.45
1:A:625:G:H2'	1:A:626:U:H6	1.81	0.45
10:J:8:LEU:HD13	10:J:19:SER:OG	2.16	0.45
1:A:708:C:H2'	1:A:709:G:H8	1.81	0.45
1:A:1346:A:C5	7:G:10:ARG:NH2	2.84	0.45
1:A:1305:G:O2'	1:A:1331:G:N2	2.42	0.45
1:A:390:C:H2'	1:A:391:G:C8	2.52	0.45
13:M:9:ILE:HA	13:M:10:PRO:HD3	1.47	0.45
16:P:67:THR:H	16:P:70:ALA:HB3	1.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:542:G:OP1	4:D:10:ARG:NH2	2.50	0.45
13:M:49:THR:OG1	13:M:52:GLU:HG3	2.17	0.45
1:A:1206:G:C6	1:A:1207:G:C6	3.04	0.45
1:A:1142:G:H2'	1:A:1143:G:O4'	2.17	0.45
1:A:684:A:C6	1:A:685:G:C6	3.05	0.45
16:P:21:VAL:O	16:P:33:ILE:HG12	2.17	0.45
1:A:1128:C:H5	1:A:1139:G:HO2'	1.64	0.45
2:B:21:ARG:HB3	2:B:39:ILE:HG12	1.98	0.45
17:Q:66:SER:OG	17:Q:67:LYS:O	2.34	0.45
1:A:797:C:O2'	1:A:798:G:H5'	2.16	0.45
16:P:6:LEU:HB3	16:P:17:TYR:HD2	1.80	0.45
12:L:24:VAL:O	12:L:26:ALA:N	2.48	0.45
1:A:69:G:C2	1:A:70:G:C8	3.04	0.45
1:A:69:G:H2'	1:A:70:G:H8	1.80	0.45
1:A:1438:G:H2'	1:A:1439:C:H6	1.82	0.45
1:A:6:G:C4	5:E:119:LEU:HD11	2.51	0.45
8:H:25:ASP:OD2	8:H:60:ARG:HG3	2.16	0.45
1:A:1452:C:HO2'	1:A:1456:G:P	2.39	0.45
1:A:941:G:C6	1:A:1343:G:C6	3.05	0.45
15:O:24:SER:O	15:O:26:GLU:N	2.50	0.45
1:A:841:U:H6	1:A:841:U:OP1	1.99	0.45
1:A:1530:G:OP1	1:A:1530:G:H4'	2.16	0.45
3:C:130:VAL:HG12	3:C:131:ARG:H	1.81	0.45
1:A:992:U:HO2'	1:A:993:G:P	2.29	0.45
13:M:70:LEU:O	13:M:74:VAL:HG23	2.16	0.45
1:A:948:C:N4	25:A:2020:HOH:O	2.49	0.45
17:Q:60:ILE:O	17:Q:62:SER:OG	2.34	0.45
1:A:775:G:C2'	1:A:776:G:H5'	2.47	0.45
1:A:1277:C:C2'	1:A:1278:U:H5'	2.46	0.45
6:F:22:GLU:OE2	6:F:82:ARG:HG2	2.17	0.45
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.52	0.45
1:A:965:A:C2	1:A:969:A:C2	3.05	0.45
1:A:519:C:H2'	1:A:520:A:C8	2.51	0.45
1:A:942:G:H2'	1:A:943:U:H6	1.82	0.45
7:G:99:LEU:HB3	7:G:103:TRP:CZ3	2.51	0.45
10:J:16:LEU:HD23	10:J:16:LEU:HA	1.75	0.45
1:A:230:G:H2'	1:A:231:G:O4'	2.17	0.45
1:A:107:G:H2'	1:A:108:G:O4'	2.17	0.45
4:D:190:ASP:OD1	4:D:190:ASP:N	2.50	0.45
1:A:1160:G:H2'	1:A:1160:G:N3	2.32	0.45
1:A:1256:A:N6	1:A:1278:U:H1'	2.22	0.45
1:A:1088:G:C6	1:A:1089:G:N7	2.84	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:65:LYS:HA	13:M:66:LEU:CB	2.45	0.45
16:P:52:ASP:OD2	16:P:55:ARG:HG2	2.16	0.45
1:A:1314:C:H2'	1:A:1315:U:C6	2.51	0.45
1:A:1510:U:H2'	1:A:1511:G:C8	2.50	0.45
1:A:1201:A:O2'	1:A:1202:G:OP2	2.18	0.45
1:A:1149:C:O2'	1:A:1280:A:N1	2.36	0.45
1:A:1062:U:H2'	1:A:1063:C:C6	2.51	0.45
1:A:750:G:N2	15:O:23:GLY:HA3	2.32	0.45
3:C:179:ARG:HH21	3:C:206:GLU:CD	2.21	0.45
1:A:1187:G:OP1	9:I:113:LYS:HE2	2.16	0.45
1:A:102:G:H2'	1:A:103:C:H6	1.81	0.45
1:A:765:G:H5''	1:A:766:A:OP1	2.17	0.45
20:T:87:LYS:O	20:T:91:LEU:HG	2.16	0.45
17:Q:45:HIS:HB2	17:Q:65:ILE:HD13	1.99	0.45
15:O:18:PHE:HB2	15:O:19:PRO:HD2	1.98	0.45
17:Q:13:ASP:OD1	17:Q:13:ASP:N	2.50	0.45
4:D:36:ARG:HG2	4:D:38:TYR:CZ	2.52	0.45
9:I:28:VAL:N	9:I:31:GLN:O	2.32	0.45
1:A:1352:C:H2'	1:A:1353:G:C8	2.51	0.45
16:P:53:VAL:O	16:P:56:ALA:N	2.50	0.45
3:C:35:GLU:O	3:C:39:ILE:HG13	2.17	0.45
1:A:403:C:P	4:D:137:SER:OG	2.75	0.45
17:Q:24:GLU:OE2	17:Q:37:LYS:HD3	2.17	0.45
1:A:127:G:HO2'	17:Q:2:PRO:N	2.14	0.45
1:A:38:G:C2	1:A:397:A:C2	3.05	0.45
1:A:877:C:H5''	8:H:88:LYS:HD3	1.99	0.45
1:A:436:C:H1'	1:A:437:U:H5'	1.99	0.45
9:I:26:VAL:CG1	9:I:61:ALA:HB3	2.45	0.45
16:P:72:ARG:HE	16:P:73:LEU:HD23	1.82	0.45
7:G:15:ASP:O	7:G:19:GLY:N	2.49	0.45
1:A:427:U:P	4:D:13:ARG:HH22	2.39	0.44
1:A:1392:G:H21	1:A:1502:A:H8	1.65	0.44
1:A:950:U:H2'	1:A:951:G:C8	2.52	0.44
1:A:1151:A:C2	1:A:1152:A:C5	3.04	0.44
7:G:72:ARG:NH1	7:G:142:GLU:OE1	2.50	0.44
1:A:21:G:H2'	1:A:22:G:C8	2.52	0.44
16:P:20:VAL:HG21	16:P:32:TYR:CG	2.52	0.44
1:A:1115:C:H1'	14:N:61:TRP:O	2.16	0.44
8:H:58:TYR:O	8:H:59:LEU:HD23	2.17	0.44
3:C:187:ALA:O	3:C:198:VAL:HG23	2.16	0.44
1:A:1261:A:H5'	1:A:1283:G:O3'	2.18	0.44
1:A:380:G:N2	1:A:384:G:C5	2.84	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:139:LEU:HD23	5:E:142:LEU:HD11	1.99	0.44
1:A:922:G:N3	1:A:1398:A:C2	2.82	0.44
9:I:45:ALA:HB1	9:I:47:LEU:N	2.31	0.44
3:C:45:LYS:O	3:C:47:LEU:N	2.48	0.44
22:Y:44:GLU:HB3	22:Y:47:GLY:C	2.38	0.44
1:A:1103:C:N3	1:A:1104:G:C8	2.85	0.44
1:A:1116:C:H2'	1:A:1117:G:H5''	1.97	0.44
1:A:690:G:C6	1:A:691:G:C6	3.05	0.44
6:F:97:PHE:O	18:R:31:LEU:HD23	2.17	0.44
22:Y:26:LYS:HD3	22:Y:82:GLU:OE2	2.17	0.44
20:T:56:MET:HG3	20:T:57:ARG:N	2.31	0.44
1:A:1372:U:C4	1:A:1373:G:C4	3.06	0.44
2:B:51:LEU:O	2:B:55:PHE:HD2	2.00	0.44
1:A:719:C:O2	18:R:50:ILE:HG12	2.17	0.44
1:A:414:A:H2'	1:A:415:A:H8	1.80	0.44
1:A:909:A:H2'	1:A:910:C:O4'	2.16	0.44
1:A:1279:A:O2'	1:A:1281:U:OP2	2.35	0.44
3:C:136:GLN:O	3:C:139:GLN:N	2.51	0.44
14:N:23:ARG:HD3	14:N:29:ARG:O	2.17	0.44
14:N:7:ILE:HG12	14:N:23:ARG:HG2	2.00	0.44
2:B:133:LYS:O	2:B:137:ARG:HG3	2.18	0.44
1:A:1321:C:H5''	1:A:1322:C:H5''	1.99	0.44
9:I:83:ARG:HA	9:I:86:VAL:HG22	1.99	0.44
1:A:685:G:C2	1:A:686:U:C4	3.05	0.44
1:A:959:A:H2'	1:A:960:U:H4'	2.00	0.44
8:H:51:VAL:HG11	8:H:60:ARG:HH11	1.81	0.44
5:E:59:GLY:O	5:E:62:ALA:HB3	2.17	0.44
1:A:105:G:H2'	1:A:106:C:C6	2.53	0.44
7:G:111:ARG:NH1	7:G:122:HIS:HB3	2.31	0.44
1:A:1279:A:H5''	1:A:1280:A:OP1	2.18	0.44
16:P:28:ARG:HH11	16:P:28:ARG:CG	2.26	0.44
4:D:193:ASP:OD2	25:D:401:HOH:O	2.21	0.44
13:M:67:GLU:HA	13:M:69:GLU:O	2.18	0.44
1:A:297:G:N2	1:A:300:A:OP2	2.49	0.44
1:A:1272:G:C6	1:A:1273:G:C5	3.06	0.44
10:J:63:PHE:HD1	14:N:57:ARG:O	2.01	0.44
17:Q:57:VAL:HA	17:Q:77:VAL:HG23	1.98	0.44
1:A:1076:C:C2	1:A:1082:G:N2	2.86	0.44
7:G:40:ALA:HB3	9:I:41:VAL:HG21	2.00	0.44
1:A:586:C:C2'	1:A:587:G:H5'	2.47	0.44
1:A:1505:G:H4'	1:A:1506:U:H5''	1.98	0.44
1:A:954:G:C5	1:A:955:U:C4	3.06	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1012:U:H2'	1:A:1013:G:O4'	2.16	0.44
16:P:3:LYS:O	16:P:21:VAL:HA	2.18	0.44
12:L:27:LEU:CB	12:L:33:ARG:HD3	2.48	0.44
1:A:1124:G:OP2	1:A:1124:G:H8	2.01	0.44
14:N:3:ARG:HB3	14:N:3:ARG:HE	1.53	0.44
1:A:1347:G:H22	1:A:1374:A:P	2.40	0.44
1:A:1262:C:H2'	1:A:1263:C:C6	2.53	0.44
2:B:42:ILE:HG21	2:B:202:PRO:O	2.17	0.44
3:C:141:VAL:HG11	3:C:202:ILE:HG12	2.00	0.44
1:A:927:G:N1	1:A:1391:U:C2	2.85	0.44
1:A:707:C:OP1	11:K:85:ARG:NH1	2.48	0.44
3:C:181:ASN:O	3:C:203:PHE:HA	2.18	0.44
1:A:520:A:N1	1:A:536:C:H1'	2.33	0.44
1:A:685:G:N2	1:A:686:U:C4	2.86	0.44
12:L:85:ILE:HD13	12:L:85:ILE:HA	1.69	0.44
1:A:1006:C:C2'	1:A:1007:C:H5'	2.48	0.44
1:A:1426:C:H2'	1:A:1427:U:C6	2.53	0.44
1:A:619:U:O2	4:D:133:VAL:HA	2.18	0.44
1:A:128:G:O2'	17:Q:3:LYS:HE2	2.18	0.44
1:A:724:G:C2	1:A:725:G:C8	3.06	0.44
1:A:820:U:H4'	1:A:821:G:OP2	2.18	0.44
1:A:1194:U:H2'	1:A:1195:C:C6	2.53	0.44
8:H:112:LEU:HB3	8:H:133:LEU:HA	2.00	0.43
3:C:11:ARG:O	3:C:14:ILE:N	2.41	0.43
1:A:56:U:H2'	1:A:57:G:H8	1.82	0.43
1:A:501:C:H1'	1:A:549:C:H1'	2.00	0.43
1:A:841:U:C5	1:A:848:C:H1'	2.53	0.43
19:S:7:LYS:HA	19:S:7:LYS:HD3	1.58	0.43
2:B:87:ARG:NH2	2:B:233:SER:HB2	2.33	0.43
1:A:1366:C:H2'	1:A:1367:C:H6	1.83	0.43
1:A:20:U:H2'	1:A:21:G:O4'	2.18	0.43
1:A:1321:C:H3'	1:A:1322:C:H5''	2.01	0.43
3:C:125:GLU:OE1	3:C:190:ARG:N	2.41	0.43
1:A:999:C:H2'	1:A:1000:U:H6	1.83	0.43
2:B:101:MET:C	2:B:102:LEU:HD12	2.39	0.43
1:A:673:G:N2	1:A:674:G:C2	2.86	0.43
1:A:814:A:H2'	1:A:816:A:H5''	1.99	0.43
1:A:333:G:H4'	20:T:16:HIS:CE1	2.53	0.43
7:G:104:LEU:HA	7:G:104:LEU:HD13	1.85	0.43
9:I:62:TYR:O	9:I:63:ILE:HG13	2.18	0.43
22:Y:29:LYS:HG3	22:Y:30:TRP:CE3	2.53	0.43
21:U:18:TYR:HD2	21:U:22:ARG:HD2	1.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:99:ALA:HB3	18:R:29:PHE:CE1	2.53	0.43
1:A:1106:G:C6	1:A:1107:C:C4	3.06	0.43
4:D:22:LYS:O	4:D:113:SER:HB3	2.18	0.43
1:A:1347:G:HO2'	1:A:1373:G:H1	1.65	0.43
1:A:10:A:OP2	5:E:126:ARG:HD2	2.17	0.43
1:A:832:C:O2'	1:A:833:U:P	2.77	0.43
1:A:622:A:C8	1:A:623:C:C5	3.06	0.43
13:M:86:CYS:SG	19:S:73:GLU:HB3	2.59	0.43
1:A:455:C:H6	1:A:455:C:O5'	2.02	0.43
14:N:23:ARG:HD2	14:N:28:GLY:C	2.38	0.43
1:A:991:U:O2'	1:A:992:U:O5'	2.34	0.43
1:A:17:U:O2'	1:A:1079:G:H1'	2.18	0.43
1:A:96:U:O2'	1:A:97:G:P	2.77	0.43
1:A:1446:U:O2'	1:A:1447:A:H3'	2.18	0.43
1:A:1073:U:OP1	5:E:57:LYS:HE3	2.19	0.43
1:A:260:G:H2'	1:A:261:U:C6	2.53	0.43
19:S:62:ILE:HA	19:S:66:MET:SD	2.58	0.43
12:L:54:LYS:N	12:L:54:LYS:HD2	2.34	0.43
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.46	0.43
10:J:36:GLY:O	10:J:38:ILE:N	2.51	0.43
1:A:1053:G:C3'	1:A:1054:C:H5'	2.49	0.43
7:G:72:ARG:H	7:G:72:ARG:HG2	1.58	0.43
3:C:180:ALA:HB1	3:C:203:PHE:CE1	2.53	0.43
1:A:509:A:H5'	4:D:54:TYR:CD2	2.53	0.43
3:C:164:ARG:HE	3:C:164:ARG:HB3	1.51	0.43
1:A:1339:A:O5'	1:A:1339:A:H8	2.02	0.43
7:G:113:GLU:HG3	7:G:118:VAL:HG12	2.00	0.43
1:A:1387:G:H2'	1:A:1388:C:C6	2.53	0.43
1:A:954:G:C6	1:A:955:U:C4	3.07	0.43
1:A:580:U:H2'	1:A:581:G:O4'	2.19	0.43
1:A:790:A:H61	1:A:1498:U:P	2.42	0.43
3:C:23:TYR:CG	3:C:24:ALA:N	2.87	0.43
1:A:509:A:O4'	4:D:58:LEU:HD12	2.18	0.43
1:A:1375:A:H4'	7:G:29:LYS:NZ	2.34	0.43
1:A:7:G:H5'	1:A:298:A:O4'	2.18	0.43
2:B:98:LEU:HA	2:B:98:LEU:HD23	1.76	0.43
1:A:968:A:C8	1:A:1062:U:H4'	2.54	0.43
1:A:1002:G:H2'	1:A:1003:G:O4'	2.18	0.43
1:A:1287:A:C6	1:A:1288:A:C6	3.07	0.43
1:A:1088:G:C5	1:A:1089:G:N7	2.87	0.43
4:D:110:PHE:CD1	4:D:110:PHE:N	2.81	0.43
4:D:18:LYS:HZ2	4:D:31:CYS:HB3	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:604:G:C2	1:A:635:G:C4	3.07	0.43
1:A:1104:G:C6	1:A:1105:A:C5	3.07	0.43
14:N:41:ARG:HG3	14:N:42:ILE:N	2.34	0.43
1:A:436:C:O2'	1:A:437:U:P	2.76	0.43
13:M:66:LEU:HD23	13:M:66:LEU:N	2.34	0.43
1:A:1492:A:OP1	12:L:47:LYS:HE3	2.18	0.43
1:A:1132:C:H2'	1:A:1133:G:C8	2.53	0.43
3:C:24:ALA:HB3	3:C:29:TYR:HB2	1.99	0.43
17:Q:57:VAL:HG12	17:Q:76:LEU:HD12	2.00	0.43
2:B:56:ARG:O	2:B:60:ASP:HB2	2.19	0.43
1:A:516:U:C5	1:A:517:G:C6	3.06	0.43
1:A:397:A:N3	1:A:397:A:H3'	2.33	0.43
1:A:584:G:H5'	17:Q:91:ARG:NH2	2.32	0.42
1:A:1084:G:C6	1:A:1085:U:C4	3.07	0.42
1:A:1516:G:N1	1:A:1519:A:OP2	2.52	0.42
1:A:375:U:OP1	16:P:69:THR:HG21	2.19	0.42
11:K:20:TYR:HB2	11:K:31:THR:HG23	2.01	0.42
14:N:40:CYS:SG	14:N:43:CYS:HB2	2.58	0.42
1:A:1349:A:C2'	1:A:1350:A:H8	2.28	0.42
1:A:983:A:H1'	1:A:1049:U:O2	2.18	0.42
9:I:43:ALA:HA	9:I:74:ILE:HG21	1.99	0.42
1:A:1147:C:H2'	9:I:16:ARG:HH12	1.84	0.42
13:M:69:GLU:O	13:M:71:ARG:N	2.47	0.42
1:A:559:A:H4'	1:A:560:U:H3'	2.01	0.42
1:A:1138:G:O2'	1:A:1140:C:OP1	2.30	0.42
1:A:1304:G:C6	1:A:1305:G:N1	2.87	0.42
1:A:1456:G:HO2'	20:T:39:LYS:NZ	2.15	0.42
13:M:48:LEU:O	13:M:53:VAL:HG23	2.19	0.42
1:A:751:U:H4'	15:O:24:SER:HB2	2.01	0.42
9:I:67:GLY:O	9:I:73:GLN:NE2	2.37	0.42
1:A:617:G:H4'	16:P:44:THR:O	2.18	0.42
1:A:174:C:H2'	1:A:175:C:C6	2.54	0.42
15:O:18:PHE:CD1	15:O:18:PHE:C	2.92	0.42
3:C:66:VAL:O	3:C:68:VAL:HG23	2.19	0.42
1:A:979:C:H42	14:N:18:VAL:HB	1.85	0.42
1:A:538:G:P	12:L:115:LYS:H	2.41	0.42
1:A:1442(A):G:N7	1:A:1442(B):A:C2	2.86	0.42
1:A:1441:G:N2	1:A:1459:C:C6	2.83	0.42
1:A:1131:G:H2'	1:A:1132:C:C6	2.54	0.42
1:A:1274:G:H21	1:A:1275:A:H62	1.67	0.42
1:A:1458:G:H5''	20:T:31:SER:CB	2.50	0.42
1:A:1143:G:H2'	1:A:1144:G:H8	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.83	0.42
1:A:982:U:OP1	1:A:982:U:H6	2.02	0.42
4:D:176:LEU:HD12	4:D:177:ASP:H	1.85	0.42
3:C:139:GLN:HG3	3:C:143:GLU:OE1	2.20	0.42
1:A:1456:G:N1	20:T:51:GLU:OE1	2.51	0.42
1:A:1097:C:H1'	1:A:1169:A:C2	2.54	0.42
1:A:428:G:HO2'	1:A:429:U:P	2.42	0.42
15:O:9:GLN:HA	15:O:12:ILE:HD12	2.01	0.42
4:D:31:CYS:HB3	4:D:33:MET:HB2	2.00	0.42
5:E:31:LEU:HD23	5:E:45:PHE:HB2	2.01	0.42
7:G:13:GLN:HA	7:G:14:PRO:HD3	1.86	0.42
4:D:159:ARG:O	4:D:163:GLU:N	2.51	0.42
16:P:14:ASN:OD1	16:P:16:HIS:CE1	2.72	0.42
1:A:1332:A:H8	1:A:1332:A:O5'	2.02	0.42
1:A:1163:C:N3	1:A:1174:G:C2	2.88	0.42
1:A:1236:A:O2'	1:A:1304:G:H4'	2.20	0.42
1:A:1323:G:H2'	1:A:1324:A:C8	2.55	0.42
1:A:974:A:H8	1:A:974:A:OP1	2.02	0.42
1:A:435:C:H42	1:A:436:C:H41	1.67	0.42
1:A:990:C:O2	1:A:1215:G:N1	2.37	0.42
1:A:1112:C:O2	3:C:179:ARG:HG2	2.18	0.42
2:B:41:ILE:HD13	2:B:41:ILE:HA	1.91	0.42
2:B:12:GLU:O	2:B:16:HIS:HB2	2.20	0.42
1:A:450:G:OP1	16:P:43:LYS:NZ	2.53	0.42
1:A:527:G:O2'	1:A:535:A:N1	2.40	0.42
5:E:41:VAL:HG23	5:E:67:VAL:HG13	2.02	0.42
1:A:728:A:N1	1:A:729:A:C6	2.88	0.42
22:Y:58:ASN:HB2	22:Y:88:LEU:HD22	2.00	0.42
9:I:27:THR:HG1	9:I:28:VAL:H	1.66	0.42
1:A:1220:G:H1'	19:S:52:TYR:CE2	2.54	0.42
1:A:1442(A):G:C5	1:A:1442(B):A:C6	3.07	0.42
1:A:1443:G:N3	1:A:1443:G:H2'	2.35	0.42
1:A:1461:G:O5'	1:A:1461:G:H8	2.03	0.42
1:A:1065:U:H3	1:A:1109:C:H5''	1.84	0.42
1:A:953:G:C2	1:A:954:G:H1'	2.55	0.42
1:A:474:G:H2'	1:A:475:G:C8	2.55	0.42
11:K:99:GLN:HG2	11:K:105:VAL:HG11	2.01	0.42
1:A:1314:C:H2'	1:A:1315:U:H6	1.85	0.42
3:C:43:LEU:O	3:C:47:LEU:HB2	2.19	0.42
1:A:573:A:P	25:A:1923:HOH:O	2.72	0.42
2:B:35:GLU:HA	2:B:39:ILE:O	2.20	0.42
1:A:1492:A:H2'	1:A:1492:A:N3	2.35	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:500:G:H2'	1:A:501:C:C6	2.55	0.42
1:A:756:C:H2'	1:A:757:U:O4'	2.20	0.42
3:C:40:ARG:O	3:C:44:GLU:HB2	2.19	0.42
1:A:250:A:H4'	1:A:251:G:O5'	2.19	0.42
19:S:33:THR:HA	19:S:34:TRP:CE3	2.55	0.42
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.69	0.42
7:G:81:GLY:O	7:G:83:ALA:N	2.53	0.42
13:M:106:ASN:HB3	13:M:107:ALA:H	1.38	0.42
1:A:1490:C:H2'	1:A:1491:G:O4'	2.19	0.42
7:G:70:LYS:HA	7:G:71:PRO:HD2	1.81	0.42
1:A:1324:A:C4'	1:A:1362:C:H4'	2.50	0.42
1:A:391:G:C6	1:A:392:G:C5	3.08	0.42
1:A:1442:G:O6	1:A:1442(A):G:O6	2.38	0.42
2:B:185:ILE:HA	2:B:199:TYR:O	2.18	0.42
1:A:1386:G:C2	1:A:1387:G:N7	2.88	0.42
8:H:123:GLU:O	8:H:127:LEU:HB2	2.19	0.42
3:C:92:ALA:HB1	3:C:97:LYS:O	2.19	0.42
1:A:1272:G:H5'	1:A:1273:G:OP2	2.19	0.42
1:A:279:A:OP2	17:Q:95:TYR:OH	2.31	0.42
10:J:16:LEU:HD13	10:J:70:ARG:HG3	2.00	0.42
5:E:78:HIS:CD2	5:E:142:LEU:HD23	2.55	0.42
12:L:110:VAL:HG23	12:L:120:TYR:HB3	2.02	0.42
1:A:1203:C:H2'	1:A:1204:A:O4'	2.20	0.42
11:K:22:HIS:HB3	11:K:29:ILE:HB	2.02	0.42
1:A:1357:A:C8	1:A:1358:U:C5	3.07	0.42
1:A:1122:U:H2'	1:A:1123:A:O4'	2.19	0.42
1:A:192:U:C4'	20:T:102:GLY:HA2	2.50	0.42
1:A:1316:G:H21	1:A:1318:A:H3'	1.85	0.42
1:A:404:U:H2'	1:A:405:U:H6	1.85	0.42
1:A:1262:C:N3	1:A:1273:G:N2	2.68	0.42
10:J:35:SER:OG	10:J:73:ASP:HB2	2.20	0.42
1:A:604:G:H2'	1:A:605:U:O4'	2.20	0.42
1:A:1010:G:O6	1:A:1019:C:N3	2.53	0.42
11:K:62:GLN:NE2	11:K:93:GLN:OE1	2.50	0.42
1:A:380:G:C2	1:A:384:G:C6	3.08	0.42
22:Y:58:ASN:H	22:Y:58:ASN:ND2	2.18	0.42
1:A:109:A:H2'	1:A:326:G:N2	2.34	0.42
1:A:1058:G:N2	10:J:53:PRO:HG3	2.34	0.42
1:A:124:G:H4'	1:A:291:C:O2'	2.18	0.42
20:T:18:GLN:O	20:T:22:ARG:HG3	2.20	0.42
9:I:13:ALA:HB2	9:I:68:GLY:HA3	2.01	0.42
1:A:1121:U:C4	1:A:1122:U:C5	3.08	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1442(A):G:C5	1:A:1442(B):A:C5	3.08	0.41
1:A:1004:A:C5'	1:A:1025:U:C5	3.03	0.41
1:A:1452:C:H6	1:A:1452:C:H2'	1.67	0.41
1:A:920:U:C2	1:A:921:U:C5	3.08	0.41
7:G:72:ARG:HH12	7:G:138:LYS:NZ	2.18	0.41
3:C:36:ASP:OD1	3:C:57:ILE:HG21	2.20	0.41
1:A:1310:G:H2'	1:A:1311:G:C8	2.55	0.41
1:A:460:G:O6	1:A:470:C:H5''	2.20	0.41
11:K:48:ILE:HD11	11:K:64:ALA:HA	2.01	0.41
1:A:911:U:OP2	12:L:97:ARG:NH1	2.53	0.41
4:D:88:VAL:O	4:D:92:VAL:HG23	2.18	0.41
12:L:59:ARG:HG2	12:L:65:GLU:HB2	2.01	0.41
1:A:925:G:H1'	1:A:1502:A:C4	2.55	0.41
1:A:472:A:O3'	16:P:81:ARG:HA	2.19	0.41
14:N:29:ARG:HE	14:N:40:CYS:HB2	1.85	0.41
1:A:1060:C:C2'	1:A:1061:G:H5'	2.50	0.41
4:D:22:LYS:HG3	4:D:26:CYS:SG	2.60	0.41
1:A:1285:A:H4'	1:A:1286:A:O5'	2.20	0.41
1:A:1090:U:H1'	1:A:1170:A:H2	1.85	0.41
1:A:706:A:H2'	1:A:707:C:H5'	2.02	0.41
1:A:429:U:H4'	1:A:430:A:O5'	2.19	0.41
14:N:5:ALA:O	14:N:9:LYS:HB2	2.20	0.41
4:D:173:TRP:NE1	4:D:174:LEU:HG	2.35	0.41
1:A:1338:G:H2'	1:A:1339:A:C8	2.55	0.41
1:A:163:C:H2'	1:A:164:U:O4'	2.20	0.41
1:A:1038:C:H2'	1:A:1039:C:O4'	2.20	0.41
4:D:171:GLY:HA2	4:D:172:PRO:HD3	1.89	0.41
11:K:103:LEU:HA	11:K:103:LEU:HD23	1.91	0.41
1:A:203:U:OP2	1:A:203:U:H2'	2.20	0.41
1:A:1148:U:OP1	9:I:7:THR:HG21	2.20	0.41
1:A:1298:C:H4'	1:A:1299:A:C4	2.54	0.41
1:A:222:U:C2	1:A:223:U:C5	3.08	0.41
1:A:1192:C:C5	1:A:1193:G:C8	3.08	0.41
3:C:181:ASN:N	3:C:205:GLY:O	2.52	0.41
1:A:97:G:O2'	1:A:98:G:OP2	2.31	0.41
2:B:180:LEU:HA	2:B:180:LEU:HD23	1.85	0.41
1:A:373:A:C2	1:A:374:A:C8	3.09	0.41
14:N:29:ARG:NE	14:N:40:CYS:HB2	2.36	0.41
1:A:1442:G:C2'	1:A:1442(A):G:H5'	2.50	0.41
1:A:1118:C:H2'	1:A:1119:C:O4'	2.20	0.41
1:A:1169:A:C2	1:A:1170:A:C4	3.08	0.41
5:E:53:LEU:H	5:E:53:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:537:G:H5''	12:L:113:ARG:NH1	2.35	0.41
19:S:48:THR:HA	19:S:60:VAL:O	2.21	0.41
6:F:61:LEU:HD23	6:F:63:TYR:OH	2.21	0.41
1:A:375:U:O3'	16:P:6:LEU:HB2	2.20	0.41
4:D:19:LEU:HA	4:D:19:LEU:HD12	1.87	0.41
18:R:31:LEU:HD23	18:R:31:LEU:O	2.20	0.41
1:A:1296:C:H5'	1:A:1297:C:OP2	2.20	0.41
1:A:1288:A:H1'	1:A:1352:C:O2'	2.21	0.41
1:A:1370:G:N7	9:I:109:VAL:HG11	2.35	0.41
1:A:166:G:H2'	1:A:167:G:H8	1.85	0.41
3:C:180:ALA:HB1	3:C:203:PHE:HE1	1.85	0.41
1:A:615:C:H2'	1:A:616:G:O4'	2.20	0.41
3:C:9:GLY:HA3	14:N:49:HIS:HA	2.01	0.41
7:G:46:ALA:HB2	7:G:117:ALA:O	2.20	0.41
6:F:49:ALA:HB2	18:R:78:LEU:O	2.21	0.41
2:B:111:ARG:HH11	2:B:111:ARG:HA	1.85	0.41
3:C:139:GLN:O	3:C:143:GLU:HB2	2.20	0.41
3:C:151:VAL:HA	3:C:199:LYS:O	2.21	0.41
3:C:52:LEU:HB2	3:C:69:HIS:O	2.19	0.41
1:A:1012:U:C4	1:A:1013:G:C5	3.09	0.41
16:P:52:ASP:HB3	16:P:55:ARG:HB2	2.01	0.41
1:A:113:G:H2'	1:A:114:U:C6	2.56	0.41
4:D:94:LEU:HA	4:D:97:LEU:HD12	2.02	0.41
1:A:975:A:H5'	1:A:975:A:H8	1.86	0.41
20:T:4:LYS:HA	20:T:4:LYS:HD3	1.95	0.41
1:A:1371:G:OP1	9:I:11:LYS:O	2.39	0.41
1:A:376:G:P	16:P:67:THR:HG21	2.60	0.41
1:A:22:G:H4'	1:A:885:G:C8	2.55	0.41
1:A:44:G:H2'	1:A:45:U:O4'	2.21	0.41
1:A:659:U:C2'	1:A:660:G:H5'	2.51	0.41
6:F:10:LEU:HD21	6:F:61:LEU:HD22	2.02	0.41
1:A:648:A:H2'	1:A:649:G:C8	2.56	0.41
17:Q:86:GLU:O	17:Q:90:ILE:HG12	2.20	0.41
8:H:38:ILE:HD12	8:H:118:VAL:HG12	2.03	0.41
1:A:678:U:H2'	1:A:679:C:C6	2.56	0.41
1:A:538:G:P	12:L:115:LYS:HB2	2.60	0.41
1:A:149:A:O2'	1:A:150:C:C6	2.67	0.41
1:A:936:C:H2'	1:A:937:A:O4'	2.20	0.41
1:A:741:G:H2'	1:A:742:G:O4'	2.21	0.41
16:P:72:ARG:NH1	16:P:72:ARG:HG3	2.36	0.41
2:B:71:VAL:HG13	2:B:93:VAL:HG21	2.02	0.41
1:A:200:G:H1	1:A:217:C:H42	1.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:111:ARG:HD3	2:B:111:ARG:HA	1.83	0.41
12:L:8:ASN:O	12:L:12:ARG:HG3	2.21	0.41
1:A:546:G:OP1	4:D:73:ARG:HB2	2.21	0.41
2:B:179:LYS:HA	8:H:72:PRO:HG3	2.02	0.41
7:G:68:ASN:ND2	7:G:128:ALA:O	2.53	0.41
22:Y:23:ARG:HG3	22:Y:78:ILE:HG13	2.03	0.41
2:B:185:ILE:HG22	2:B:199:TYR:CD1	2.55	0.41
1:A:1066:C:O2'	1:A:1067:A:H5'	2.20	0.41
22:Y:17:ARG:O	22:Y:20:VAL:HG12	2.21	0.41
1:A:872:A:C4	1:A:874:G:N7	2.89	0.41
9:I:74:ILE:HA	9:I:77:ILE:HD12	2.03	0.41
1:A:1089:G:H1	1:A:1096:C:N4	2.14	0.41
1:A:1493:A:C2	1:A:1494:G:C8	3.09	0.41
1:A:473:G:H2'	1:A:474:G:C8	2.51	0.41
19:S:35:SER:O	19:S:37:ARG:N	2.54	0.41
1:A:542:G:H2'	1:A:543:C:C6	2.54	0.41
1:A:1238:A:OP1	1:A:1335:C:H1'	2.20	0.41
1:A:561:U:O2'	1:A:562:C:P	2.78	0.41
1:A:1055:A:O2'	3:C:161:GLU:O	2.35	0.41
8:H:21:LYS:O	8:H:63:LEU:HD23	2.21	0.41
2:B:71:VAL:HG13	2:B:93:VAL:HG23	2.03	0.41
16:P:48:TRP:CD1	16:P:48:TRP:N	2.88	0.41
15:O:29:VAL:HG11	15:O:81:LEU:HD21	2.03	0.41
1:A:1365:G:H5'	25:A:2159:HOH:O	2.21	0.41
1:A:1380:U:C2	7:G:3:ARG:NH1	2.89	0.41
1:A:134:A:H61	16:P:25:ARG:NH1	2.18	0.41
3:C:6:HIS:HD2	3:C:7:PRO:HD2	1.86	0.41
9:I:106:ALA:O	9:I:108:VAL:HG23	2.20	0.41
13:M:13:LYS:O	13:M:18:ALA:HB2	2.21	0.41
1:A:443:C:H2'	1:A:444:C:H6	1.86	0.41
3:C:46:GLU:CD	3:C:46:GLU:H	2.24	0.41
1:A:1299:A:C6	1:A:1301:U:C2	3.09	0.41
9:I:37:PHE:HB3	9:I:43:ALA:HB1	2.02	0.41
1:A:1187:G:H3'	1:A:1188:A:H8	1.85	0.41
8:H:49:GLU:OE2	8:H:62:TYR:OH	2.39	0.41
1:A:977:A:N1	1:A:1224:G:C8	2.89	0.41
1:A:1410:G:H2'	1:A:1411:C:H6	1.86	0.41
1:A:1338:G:C2	1:A:1339:A:C4	3.09	0.41
1:A:1338:G:C6	1:A:1339:A:C6	3.09	0.41
7:G:46:ALA:O	7:G:50:ILE:N	2.48	0.41
15:O:15:PHE:CE2	15:O:84:LYS:HD2	2.56	0.41
1:A:547:A:H5'	25:A:2177:HOH:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1246:C:H2'	1:A:1247:U:H6	1.86	0.40
1:A:1367:C:N3	1:A:1368:G:C8	2.89	0.40
1:A:983:A:H3'	1:A:983:A:N3	2.36	0.40
1:A:1434:A:H2'	1:A:1435:G:O4'	2.21	0.40
3:C:35:GLU:HG2	3:C:36:ASP:N	2.35	0.40
1:A:1133:G:H2'	1:A:1134:G:C8	2.56	0.40
1:A:453:A:C6	1:A:454:C:C4	3.09	0.40
12:L:32:PHE:HB3	12:L:84:LEU:HD11	2.03	0.40
1:A:116:A:H61	1:A:313:A:H1'	1.85	0.40
1:A:1479:C:H2'	1:A:1480:G:H8	1.85	0.40
5:E:95:ALA:HB1	5:E:96:PRO:HD2	2.02	0.40
1:A:668:G:O4'	15:O:49:ASP:HB2	2.20	0.40
15:O:3:ILE:HD13	15:O:3:ILE:H	1.85	0.40
7:G:90:GLU:CD	7:G:90:GLU:H	2.24	0.40
1:A:1088:G:C6	1:A:1089:G:C5	3.10	0.40
1:A:1492:A:H3'	1:A:1493:A:O4'	2.21	0.40
13:M:52:GLU:O	13:M:56:LEU:HB2	2.20	0.40
3:C:52:LEU:CB	3:C:70:VAL:HA	2.51	0.40
11:K:45:GLY:O	11:K:50:TYR:HB2	2.21	0.40
1:A:116:A:OP2	25:A:1951:HOH:O	2.22	0.40
3:C:19:GLU:HB2	3:C:40:ARG:HH22	1.86	0.40
3:C:109:PRO:O	3:C:112:SER:HB3	2.22	0.40
17:Q:85:VAL:O	17:Q:89:LEU:HG	2.22	0.40
15:O:50:HIS:O	15:O:53:HIS:HB3	2.21	0.40
5:E:18:ARG:O	5:E:24:ARG:HB2	2.22	0.40
4:D:196:LEU:N	4:D:196:LEU:HD12	2.36	0.40
1:A:926:G:O4'	22:Y:91:LYS:HE2	2.21	0.40
1:A:1442:G:C8	1:A:1442(A):G:C4	3.10	0.40
1:A:1062:U:H2'	1:A:1063:C:C5	2.56	0.40
7:G:56:GLN:HB2	7:G:57:GLU:H	1.59	0.40
7:G:148:ASN:HD22	7:G:151:TYR:HD1	1.66	0.40
13:M:44:ARG:HB2	13:M:47:ASP:OD2	2.21	0.40
17:Q:87:LYS:HD3	17:Q:87:LYS:HA	1.82	0.40
15:O:74:ASP:HA	15:O:75:PRO:HD2	1.84	0.40
4:D:8:VAL:HG22	4:D:21:LEU:CD1	2.51	0.40
13:M:30:ALA:O	13:M:34:LEU:HG	2.21	0.40
1:A:189(C):C:H2'	1:A:189(D):C:O4'	2.20	0.40
11:K:21:ILE:HB	11:K:84:VAL:HG22	2.03	0.40
1:A:1150:U:C4	1:A:1151:A:N7	2.90	0.40
1:A:1094:G:OP1	25:A:2096:HOH:O	2.21	0.40
1:A:953:G:C6	1:A:954:G:C5	3.10	0.40
1:A:1350:A:H2'	1:A:1351:U:C6	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1118:C:OP1	9:I:9:ARG:NH1	2.36	0.40
1:A:1189:C:H4'	3:C:10:PHE:CE1	2.57	0.40
5:E:90:VAL:O	5:E:120:THR:HA	2.21	0.40
1:A:930:C:H2'	1:A:931:C:H5'	2.04	0.40
1:A:257:G:H2'	1:A:258:G:O4'	2.21	0.40
20:T:41:ILE:HD12	20:T:42:GLN:N	2.36	0.40
1:A:66:G:OP1	1:A:66:G:H8	2.05	0.40
1:A:1245:A:C6	1:A:1246:C:C4	3.09	0.40
1:A:1356:G:N2	1:A:1367:C:C2	2.89	0.40
1:A:1309:G:O3'	13:M:77:ASN:ND2	2.54	0.40
1:A:790:A:H1'	22:Y:29:LYS:O	2.21	0.40
1:A:93:G:H1'	1:A:96:U:H5'	2.04	0.40
1:A:130:A:O2'	1:A:131:C:O5'	2.30	0.40
1:A:658:G:C6	1:A:659:U:C4	3.09	0.40
5:E:89:ILE:HD13	5:E:90:VAL:N	2.37	0.40
1:A:858:G:O6	1:A:869:G:H3'	2.21	0.40
12:L:27:LEU:CB	12:L:62:SER:HB3	2.51	0.40
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.74	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	233/256 (91%)	187 (80%)	43 (18%)	3 (1%)	18	43
3	C	204/239 (85%)	169 (83%)	31 (15%)	4 (2%)	11	28
4	D	206/209 (99%)	182 (88%)	23 (11%)	1 (0%)	38	70
5	E	146/162 (90%)	130 (89%)	15 (10%)	1 (1%)	30	62
6	F	97/101 (96%)	95 (98%)	2 (2%)	0	100	100
7	G	153/156 (98%)	130 (85%)	22 (14%)	1 (1%)	30	62
8	H	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
9	I	123/128 (96%)	104 (85%)	14 (11%)	5 (4%)	4	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	94/105 (90%)	72 (77%)	18 (19%)	4 (4%)	4	8
11	K	112/129 (87%)	104 (93%)	8 (7%)	0	100	100
12	L	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	27	58
13	M	110/126 (87%)	86 (78%)	18 (16%)	6 (6%)	3	4
14	N	58/61 (95%)	49 (84%)	5 (9%)	4 (7%)	2	2
15	O	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	P	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	18	43
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	R	66/88 (75%)	56 (85%)	10 (15%)	0	100	100
19	S	76/93 (82%)	57 (75%)	18 (24%)	1 (1%)	18	43
20	T	102/106 (96%)	79 (78%)	20 (20%)	3 (3%)	7	16
21	U	21/27 (78%)	16 (76%)	5 (24%)	0	100	100
22	Y	92/119 (77%)	87 (95%)	5 (5%)	0	100	100
All	All	2412/2657 (91%)	2082 (86%)	295 (12%)	35 (2%)	15	38

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	26	LYS
3	C	67	THR
3	C	101	LEU
13	M	7	VAL
13	M	45	VAL
14	N	13	THR
14	N	14	PRO
20	T	6	PRO
10	J	94	VAL
13	M	50	GLU
13	M	95	GLY
16	P	53	VAL
9	I	54	ASP
12	L	26	ALA
13	M	10	PRO
14	N	59	ALA
14	N	60	SER
9	I	88	TYR
9	I	119	ALA

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Mol	Chain	Res	Type
19	S	36	ARG
20	T	8	ARG
20	T	9	ASN
2	B	10	LEU
5	E	146	ALA
10	J	56	HIS
13	M	49	THR
9	I	103	THR
2	B	239	VAL
7	G	55	GLY
9	I	21	PRO
10	J	34	VAL
2	B	194	PRO
3	C	76	VAL
4	D	28	SER
10	J	90	LEU

### 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	181/220 (82%)	151 (83%)	30 (17%)	3	8
3	C	114/188 (61%)	86 (75%)	28 (25%)	1	3
4	D	142/181 (78%)	120 (84%)	22 (16%)	4	10
5	E	108/123 (88%)	94 (87%)	14 (13%)	6	15
6	F	75/90 (83%)	65 (87%)	10 (13%)	6	14
7	G	103/127 (81%)	83 (81%)	20 (19%)	2	5
8	H	104/119 (87%)	88 (85%)	16 (15%)	4	10
9	I	62/99 (63%)	53 (86%)	9 (14%)	5	12
10	J	52/92 (56%)	40 (77%)	12 (23%)	1	3
11	K	81/99 (82%)	73 (90%)	8 (10%)	11	26
12	L	91/109 (84%)	85 (93%)	6 (7%)	24	50
13	M	62/101 (61%)	45 (73%)	17 (27%)	0	2
14	N	45/50 (90%)	33 (73%)	12 (27%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	77/80 (96%)	64 (83%)	13 (17%)	3	8
16	P	65/74 (88%)	51 (78%)	14 (22%)	1	4
17	Q	93/97 (96%)	81 (87%)	12 (13%)	6	15
18	R	49/77 (64%)	40 (82%)	9 (18%)	2	6
19	S	44/80 (55%)	32 (73%)	12 (27%)	0	2
20	T	72/82 (88%)	61 (85%)	11 (15%)	4	10
21	U	14/22 (64%)	11 (79%)	3 (21%)	1	4
22	Y	79/104 (76%)	63 (80%)	16 (20%)	2	5
All	All	1713/2214 (77%)	1419 (83%)	294 (17%)	3	7

All (294) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	24	TRP
2	B	67	THR
2	B	75	LYS
2	B	80	ILE
2	B	87	ARG
2	B	93	VAL
2	B	94	ASN
2	B	97	TRP
2	B	111	ARG
2	B	126	GLU
2	B	139	LYS
2	B	150	SER
2	B	158	LEU
2	B	160	ASP
2	B	170	GLU
2	B	175	ARG
2	B	185	ILE
2	B	187	LEU
2	B	198	ASP
2	B	200	ILE
2	B	205	ASP
2	B	221	LEU

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Mol	Chain	Res	Type
2	B	224	GLN
2	B	231	GLU
2	B	238	LEU
2	B	240	GLN
3	C	8	ILE
3	C	19	GLU
3	C	20	SER
3	C	29	TYR
3	C	30	ARG
3	C	35	GLU
3	C	40	ARG
3	C	46	GLU
3	C	47	LEU
3	C	49	SER
3	C	52	LEU
3	C	55	VAL
3	C	102	ASN
3	C	103	VAL
3	C	128	PHE
3	C	132	ARG
3	C	136	GLN
3	C	140	ARG
3	C	143	GLU
3	C	152	ILE
3	C	162	GLN
3	C	164	ARG
3	C	165	THR
3	C	167	TRP
3	C	178	LEU
3	C	179	ARG
3	C	192	THR
3	C	196	LEU
4	D	8	VAL
4	D	15	GLU
4	D	19	LEU
4	D	28	SER
4	D	31	CYS
4	D	36	ARG
4	D	53	ASP
4	D	58	LEU
4	D	65	ARG
4	D	83	SER

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Mol	Chain	Res	Type
4	D	106	TYR
4	D	110	PHE
4	D	120	LEU
4	D	122	ARG
4	D	127	THR
4	D	135	LEU
4	D	158	ILE
4	D	170	VAL
4	D	181	MET
4	D	188	LEU
4	D	194	LEU
4	D	196	LEU
5	E	12	LEU
5	E	31	LEU
5	E	34	VAL
5	E	41	VAL
5	E	47	LYS
5	E	65	ASN
5	E	76	ILE
5	E	78	HIS
5	E	89	ILE
5	E	91	LEU
5	E	93	PRO
5	E	137	GLU
5	E	144	THR
5	E	147	ASP
6	F	15	ASP
6	F	36	ARG
6	F	40	VAL
6	F	55	ASP
6	F	64	GLN
6	F	69	GLU
6	F	70	ASP
6	F	72	VAL
6	F	75	LEU
6	F	82	ARG
7	G	10	ARG
7	G	12	LEU
7	G	22	LEU
7	G	32	ARG
7	G	41	ARG
7	G	47	CYS

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Mol	Chain	Res	Type
7	G	56	GLN
7	G	57	GLU
7	G	61	VAL
7	G	72	ARG
7	G	80	VAL
7	G	104	LEU
7	G	110	GLN
7	G	114	ARG
7	G	124	LEU
7	G	135	VAL
7	G	143	ARG
7	G	144	MET
7	G	146	GLU
7	G	155	ARG
8	H	21	LYS
8	H	25	ASP
8	H	26	VAL
8	H	29	SER
8	H	52	ASP
8	H	63	LEU
8	H	78	GLN
8	H	83	ILE
8	H	84	ARG
8	H	85	ARG
8	H	109	ILE
8	H	112	LEU
8	H	115	SER
8	H	121	ASP
8	H	127	LEU
8	H	133	LEU
9	I	7	THR
9	I	14	VAL
9	I	40	LEU
9	I	64	THR
9	I	87	GLN
9	I	104	ARG
9	I	105	ASP
9	I	109	VAL
9	I	117	HIS
10	J	8	LEU
10	J	33	GLN
10	J	34	VAL

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Mol	Chain	Res	Type
10	J	35	SER
10	J	44	VAL
10	J	49	VAL
10	J	55	LYS
10	J	62	HIS
10	J	67	THR
10	J	94	VAL
10	J	95	GLU
10	J	96	ILE
11	K	31	THR
11	K	48	ILE
11	K	63	LEU
11	K	84	VAL
11	K	96	ARG
11	K	104	GLN
11	K	109	VAL
11	K	114	VAL
12	L	33	ARG
12	L	43	VAL
12	L	53	ARG
12	L	60	LEU
12	L	84	LEU
12	L	97	ARG
13	M	4	ILE
13	M	15	VAL
13	M	22	ILE
13	M	23	TYR
13	M	27	LYS
13	M	40	ASN
13	M	49	THR
13	M	55	ARG
13	M	56	LEU
13	M	60	VAL
13	M	64	TRP
13	M	77	ASN
13	M	92	HIS
13	M	104	ARG
13	M	108	ARG
13	M	109	THR
13	M	110	ARG
14	N	3	ARG
14	N	4	LYS

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Mol	Chain	Res	Type
14	N	7	ILE
14	N	18	VAL
14	N	22	THR
14	N	31	ARG
14	N	32	SER
14	N	33	VAL
14	N	41	ARG
14	N	42	ILE
14	N	43	CYS
14	N	60	SER
15	O	3	ILE
15	O	10	LYS
15	O	17	ARG
15	O	24	SER
15	O	26	GLU
15	O	35	ARG
15	O	39	LEU
15	O	41	GLU
15	O	65	ARG
15	O	66	LEU
15	O	73	GLU
15	O	76	GLU
15	O	83	GLU
16	P	1	MET
16	P	2	VAL
16	P	20	VAL
16	P	28	ARG
16	P	32	TYR
16	P	33	ILE
16	P	38	TYR
16	P	45	THR
16	P	47	ASP
16	P	62	VAL
16	P	67	THR
16	P	69	THR
16	P	72	ARG
16	P	76	GLN
17	Q	9	VAL
17	Q	13	ASP
17	Q	49	GLU
17	Q	50	LYS
17	Q	53	LEU

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Mol	Chain	Res	Type
17	Q	60	ILE
17	Q	62	SER
17	Q	68	ARG
17	Q	74	LEU
17	Q	77	VAL
17	Q	82	MET
17	Q	86	GLU
18	R	21	LYS
18	R	29	PHE
18	R	31	LEU
18	R	32	ARG
18	R	58	LEU
18	R	76	LEU
18	R	82	THR
18	R	85	LEU
18	R	86	VAL
19	S	7	LYS
19	S	11	VAL
19	S	23	ASN
19	S	36	ARG
19	S	37	ARG
19	S	43	GLU
19	S	53	ASN
19	S	57	HIS
19	S	62	ILE
19	S	70	LYS
19	S	77	THR
19	S	79	THR
20	T	4	LYS
20	T	10	LEU
20	T	13	LEU
20	T	24	LEU
20	T	37	SER
20	T	39	LYS
20	T	54	LYS
20	T	56	MET
20	T	73	HIS
20	T	75	ASN
20	T	84	LEU
21	U	10	ARG
21	U	21	TYR
21	U	22	ARG

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Mol	Chain	Res	Type
22	Y	5	ILE
22	Y	16	ILE
22	Y	24	LEU
22	Y	26	LYS
22	Y	32	THR
22	Y	40	ILE
22	Y	42	SER
22	Y	58	ASN
22	Y	61	LEU
22	Y	64	SER
22	Y	74	ILE
22	Y	76	GLU
22	Y	77	LEU
22	Y	88	LEU
22	Y	93	GLU
22	Y	96	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	HIS
3	C	37	GLN
3	C	118	GLN
3	C	162	GLN
4	D	42	GLN
4	D	45	GLN
4	D	125	HIS
4	D	129	ASN
7	G	56	GLN
7	G	106	GLN
7	G	110	GLN
9	I	3	GLN
9	I	38	GLN
9	I	87	GLN
9	I	124	GLN
10	J	68	HIS
11	K	99	GLN
13	M	92	HIS
14	N	52	GLN
15	O	28	GLN
16	P	13	HIS
16	P	16	HIS

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Mol	Chain	Res	Type
22	Y	31	GLN
22	Y	33	HIS
22	Y	36	ASN
22	Y	38	HIS
22	Y	58	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1490/1522 (97%)	328 (22%)	34 (2%)

All (328) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	48	C
1	A	50	A
1	A	51	A
1	A	52	G
1	A	61	G
1	A	65	U
1	A	66	G
1	A	67	C
1	A	96	U
1	A	97	G
1	A	115	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	131	C
1	A	144	G
1	A	145	G
1	A	146	G
1	A	150	C
1	A	156	G
1	A	163	C
1	A	173	U

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Mol	Chain	Res	Type
1	A	182	U
1	A	189(G)	G
1	A	195	A
1	A	197	A
1	A	203	U
1	A	204	U
1	A	216	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	306	G
1	A	320	C
1	A	321	A
1	A	328	C
1	A	332	G
1	A	344	A
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	388	G
1	A	391	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	434	U

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Mol	Chain	Res	Type
1	A	437	U
1	A	439	A
1	A	441	A
1	A	442	C
1	A	452	A
1	A	458	C
1	A	461	A
1	A	476	G
1	A	485	G
1	A	495	A
1	A	496	A
1	A	498	U
1	A	505	G
1	A	506	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	521	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	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	588	G
1	A	596	C
1	A	617	G
1	A	623	C
1	A	630	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A

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Mol	Chain	Res	Type
1	A	673	G
1	A	687	A
1	A	688	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	749	C
1	A	755	G
1	A	764	C
1	A	777	A
1	A	793	U
1	A	794	A
1	A	817	C
1	A	827	U
1	A	828	A
1	A	829	G
1	A	833	U
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	853	G
1	A	859	A
1	A	860	A
1	A	884	U
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	944	G
1	A	954	G
1	A	959	A
1	A	961	U
1	A	966	G
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G

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Mol	Chain	Res	Type
1	A	977	A
1	A	981	U
1	A	984	C
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	995	C
1	A	998	G
1	A	1001	A
1	A	1002	G
1	A	1003	G
1	A	1005	A
1	A	1006	C
1	A	1007	C
1	A	1011	G
1	A	1019	C
1	A	1020	U
1	A	1021	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1030(B)	C
1	A	1030(C)	G
1	A	1032	G
1	A	1037	C
1	A	1038	C
1	A	1042	G
1	A	1044	A
1	A	1046	A
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1056	U
1	A	1057	G
1	A	1058	G
1	A	1062	U
1	A	1063	C
1	A	1065	U

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Mol	Chain	Res	Type
1	A	1066	C
1	A	1068	G
1	A	1073	U
1	A	1081	G
1	A	1084	G
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1108	G
1	A	1109	C
1	A	1113	C
1	A	1117	G
1	A	1119	C
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1133	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1146	A
1	A	1147	C
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1161	C
1	A	1171	G
1	A	1182	G
1	A	1184	G
1	A	1185	G
1	A	1187	G
1	A	1190	G
1	A	1194	U
1	A	1196	U
1	A	1197	G

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Mol	Chain	Res	Type
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1248	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1263	C
1	A	1267	C
1	A	1269	A
1	A	1273	G
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1295	G
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1307	U
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1324	A
1	A	1331	G
1	A	1335	C

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Mol	Chain	Res	Type
1	A	1336	C
1	A	1345	U
1	A	1346	A
1	A	1347	G
1	A	1358	U
1	A	1363	C
1	A	1363(A)	A
1	A	1364	U
1	A	1365	G
1	A	1368	G
1	A	1370	G
1	A	1379	G
1	A	1380	U
1	A	1381	U
1	A	1383	C
1	A	1397	C
1	A	1398	A
1	A	1406	U
1	A	1416	G
1	A	1419	G
1	A	1442	G
1	A	1442(A)	G
1	A	1442(B)	A
1	A	1443	G
1	A	1447	A
1	A	1452	C
1	A	1456	G
1	A	1457	G
1	A	1459	C
1	A	1460	A
1	A	1461	G
1	A	1487	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U

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Mol	Chain	Res	Type
1	A	1507	A
1	A	1508	G
1	A	1517	G
1	A	1519	A
1	A	1520	G
1	A	1529	G
1	A	1530	G

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	60	A
1	A	65	U
1	A	115	G
1	A	119	A
1	A	189(E)	U
1	A	243	A
1	A	266	G
1	A	353	A
1	A	428	G
1	A	429	U
1	A	495	A
1	A	509	A
1	A	560	U
1	A	561	U
1	A	687	A
1	A	748	C
1	A	913	A
1	A	991	U
1	A	992	U
1	A	1049	U
1	A	1061	G
1	A	1064	G
1	A	1065	U
1	A	1067	A
1	A	1129	C
1	A	1136	U
1	A	1183	A
1	A	1201	A
1	A	1256	A
1	A	1300	G

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Mol	Chain	Res	Type
1	A	1442	G
1	A	1456	G
1	A	1493	A

## 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 212 ligands modelled in this entry, 212 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	1491/1522 (97%)	0.47	81 (5%) 25 27	40, 84, 135, 175	0
2	B	235/256 (91%)	1.39	65 (27%) 1 1	80, 108, 127, 135	0
3	C	206/239 (86%)	1.13	45 (21%) 1 2	85, 109, 122, 130	0
4	D	208/209 (99%)	0.84	34 (16%) 2 3	68, 85, 103, 111	0
5	E	148/162 (91%)	0.48	20 (13%) 4 4	62, 77, 91, 105	0
6	F	99/101 (98%)	0.32	7 (7%) 16 17	62, 74, 86, 95	0
7	G	155/156 (99%)	1.28	34 (21%) 1 2	86, 102, 111, 118	0
8	H	138/138 (100%)	1.01	24 (17%) 2 2	64, 79, 87, 95	0
9	I	125/128 (97%)	2.40	57 (45%) 1 0	89, 118, 126, 133	0
10	J	96/105 (91%)	1.58	33 (34%) 1 1	95, 118, 135, 144	0
11	K	114/129 (88%)	0.52	12 (10%) 7 7	54, 77, 95, 109	0
12	L	122/132 (92%)	1.06	23 (18%) 2 2	55, 72, 85, 99	0
13	M	112/126 (88%)	2.17	46 (41%) 1 0	94, 117, 126, 134	0
14	N	60/61 (98%)	2.42	27 (45%) 1 0	99, 110, 121, 128	0
15	O	88/89 (98%)	0.99	18 (20%) 1 2	58, 77, 91, 96	0
16	P	82/88 (93%)	1.66	32 (39%) 1 1	66, 79, 94, 103	0
17	Q	99/105 (94%)	0.57	10 (10%) 7 8	60, 75, 85, 94	0
18	R	68/88 (77%)	0.92	12 (17%) 2 2	65, 76, 92, 96	0
19	S	78/93 (83%)	1.68	25 (32%) 1 1	100, 118, 130, 133	0
20	T	104/106 (98%)	1.10	23 (22%) 1 1	64, 83, 103, 119	0
21	U	23/27 (85%)	5.32	20 (86%) 0 0	97, 106, 115, 119	0
22	Y	94/119 (78%)	1.50	27 (28%) 1 1	76, 95, 113, 120	0
All	All	3945/4179 (94%)	0.95	675 (17%) 2 2	40, 89, 127, 175	0

All (675) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	U	24	ARG	14.8
7	G	2	ALA	13.2
13	M	90	LEU	12.8
2	B	93	VAL	12.1
4	D	5	ILE	11.4
9	I	101	PHE	10.5
22	Y	62	VAL	10.4
9	I	28	VAL	10.4
13	M	89	GLY	10.2
13	M	6	GLY	10.1
9	I	30	GLY	10.0
21	U	14	TRP	9.9
21	U	15	ARG	9.8
2	B	70	PHE	9.6
9	I	126	SER	9.3
13	M	87	TYR	9.3
2	B	134	GLU	9.3
12	L	63	GLY	9.2
21	U	19	GLY	9.1
10	J	5	ARG	8.9
2	B	149	LEU	8.8
13	M	88	ARG	8.8
13	M	91	ARG	8.8
7	G	5	ARG	8.7
7	G	7	ALA	8.5
19	S	31	ILE	8.3
12	L	62	SER	8.2
13	M	7	VAL	8.2
21	U	22	ARG	7.8
10	J	77	PRO	7.7
21	U	11	GLY	7.7
2	B	186	ALA	7.6
14	N	44	LEU	7.6
9	I	63	ILE	7.4
22	Y	36	ASN	7.4
8	H	57	PRO	7.4
7	G	31	MET	7.3
20	T	77	ALA	7.2
9	I	36	TYR	7.1
19	S	50	ALA	7.0
14	N	36	PHE	7.0
12	L	67	THR	6.9

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Mol	Chain	Res	Type	RSRZ
7	G	12	LEU	6.9
16	P	79	VAL	6.8
19	S	75	ALA	6.8
14	N	18	VAL	6.8
14	N	56	VAL	6.8
12	L	64	TYR	6.8
19	S	76	PRO	6.7
3	C	152	ILE	6.6
4	D	97	LEU	6.6
13	M	92	HIS	6.6
9	I	19	LEU	6.6
9	I	27	THR	6.5
21	U	16	GLY	6.5
13	M	72	ALA	6.4
21	U	23	PRO	6.4
9	I	103	THR	6.4
13	M	20	THR	6.4
22	Y	61	LEU	6.3
19	S	35	SER	6.3
19	S	74	PHE	6.3
9	I	29	ASN	6.2
2	B	133	LYS	6.2
8	H	61	VAL	6.2
9	I	62	TYR	6.1
14	N	52	GLN	6.1
1	A	1001(A)	G	6.1
9	I	42	ARG	6.0
21	U	20	LYS	6.0
13	M	86	CYS	6.0
4	D	2	GLY	5.9
2	B	201	ILE	5.9
9	I	41	VAL	5.9
9	I	45	ALA	5.8
2	B	15	VAL	5.8
9	I	32	ASP	5.8
10	J	100	THR	5.8
16	P	73	LEU	5.7
18	R	44	LEU	5.7
2	B	183	PRO	5.7
2	B	214	ILE	5.7
14	N	57	ARG	5.7
9	I	74	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
2	B	165	VAL	5.6
14	N	38	GLY	5.6
14	N	30	ALA	5.6
3	C	12	LEU	5.6
21	U	18	TYR	5.5
2	B	71	VAL	5.5
10	J	27	ALA	5.5
20	T	76	ALA	5.5
21	U	13	ILE	5.5
7	G	116	ALA	5.4
13	M	60	VAL	5.4
3	C	103	VAL	5.4
13	M	71	ARG	5.4
3	C	19	GLU	5.4
16	P	69	THR	5.4
13	M	28	ALA	5.3
19	S	82	GLY	5.3
13	M	27	LYS	5.3
9	I	114	TYR	5.3
1	A	1019	C	5.3
20	T	78	ALA	5.3
13	M	19	LEU	5.2
17	Q	68	ARG	5.2
2	B	91	PRO	5.2
2	B	92	TYR	5.1
13	M	85	GLY	5.1
2	B	188	ALA	5.1
12	L	95	GLY	5.1
3	C	184	TYR	5.1
2	B	137	ARG	5.1
7	G	39	ALA	5.1
9	I	44	VAL	5.0
21	U	21	TYR	5.0
9	I	104	ARG	5.0
1	A	1006	C	4.9
9	I	119	ALA	4.9
16	P	70	ALA	4.9
10	J	47	PHE	4.9
16	P	39	TYR	4.9
2	B	237	ALA	4.9
19	S	12	ASP	4.8
18	R	34	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
20	T	66	ALA	4.8
13	M	69	GLU	4.8
13	M	78	ILE	4.8
4	D	3	ARG	4.8
2	B	139	LYS	4.8
7	G	40	ALA	4.7
22	Y	44	GLU	4.7
15	O	45	VAL	4.7
19	S	79	THR	4.7
4	D	67	ILE	4.7
3	C	146	ALA	4.7
1	A	1039	C	4.7
9	I	35	GLU	4.7
8	H	134	ILE	4.6
3	C	87	LEU	4.6
2	B	10	LEU	4.6
13	M	101	GLN	4.6
7	G	123	GLU	4.6
2	B	187	LEU	4.6
13	M	22	ILE	4.6
22	Y	35	ILE	4.6
4	D	45	GLN	4.6
4	D	148	VAL	4.6
17	Q	66	SER	4.5
3	C	167	TRP	4.5
10	J	63	PHE	4.5
9	I	109	VAL	4.5
2	B	41	ILE	4.5
10	J	68	HIS	4.5
1	A	1003	G	4.5
15	O	3	ILE	4.4
9	I	40	LEU	4.4
2	B	68	ILE	4.4
5	E	31	LEU	4.4
9	I	66	ARG	4.4
11	K	42	TRP	4.4
3	C	169	ALA	4.3
3	C	21	ARG	4.3
1	A	1030(B)	C	4.3
13	M	93	ARG	4.3
3	C	134	ILE	4.3
20	T	33	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
3	C	173	VAL	4.3
1	A	1196	U	4.3
16	P	1	MET	4.3
9	I	96	LEU	4.3
1	A	1260	C	4.3
12	L	120	TYR	4.2
22	Y	54	ILE	4.2
14	N	19	ARG	4.2
18	R	43	PHE	4.2
9	I	115	GLY	4.2
1	A	1363	C	4.2
2	B	37	ASN	4.1
16	P	4	ILE	4.1
9	I	31	GLN	4.1
22	Y	60	VAL	4.1
15	O	74	ASP	4.1
15	O	81	LEU	4.1
6	F	93	SER	4.1
7	G	132	GLY	4.1
1	A	1223	C	4.1
9	I	18	PHE	4.1
9	I	110	GLU	4.1
4	D	66	ARG	4.1
8	H	48	TYR	4.0
8	H	13	ILE	4.0
2	B	101	MET	4.0
18	R	20	ALA	4.0
12	L	96	VAL	4.0
5	E	86	ALA	4.0
10	J	65	LEU	4.0
20	T	64	ASP	4.0
19	S	11	VAL	4.0
18	R	56	THR	4.0
3	C	172	ARG	4.0
12	L	18	VAL	3.9
13	M	94	ARG	3.9
13	M	73	GLU	3.9
19	S	80	TYR	3.9
19	S	70	LYS	3.9
9	I	75	ASP	3.9
13	M	10	PRO	3.9
20	T	29	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
14	N	45	ARG	3.9
3	C	170	GLN	3.9
4	D	4	TYR	3.9
8	H	135	CYS	3.9
2	B	154	LEU	3.9
11	K	63	LEU	3.9
7	G	4	ARG	3.9
4	D	71	SER	3.9
14	N	16	PHE	3.9
1	A	1286	A	3.8
7	G	94	ARG	3.8
12	L	17	LYS	3.8
2	B	18	GLY	3.8
14	N	37	PHE	3.8
22	Y	88	LEU	3.8
20	T	9	ASN	3.8
12	L	55	VAL	3.8
1	A	1149	C	3.8
3	C	207	VAL	3.8
19	S	29	ARG	3.8
1	A	1018	C	3.8
1	A	1353	G	3.8
10	J	67	THR	3.8
9	I	68	GLY	3.8
5	E	124	GLY	3.7
7	G	66	VAL	3.7
2	B	127	ILE	3.7
4	D	110	PHE	3.7
2	B	239	VAL	3.7
9	I	99	LEU	3.7
16	P	15	PRO	3.7
7	G	29	LYS	3.7
9	I	5	TYR	3.7
14	N	22	THR	3.7
15	O	56	LEU	3.7
15	O	85	LEU	3.7
17	Q	96	GLU	3.7
3	C	138	VAL	3.7
6	F	67	MET	3.7
10	J	86	MET	3.7
16	P	74	LEU	3.7
14	N	17	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1323	G	3.6
1	A	1385	G	3.6
7	G	3	ARG	3.6
13	M	77	ASN	3.6
2	B	185	ILE	3.6
9	I	33	PHE	3.6
22	Y	70	MET	3.6
3	C	145	GLY	3.6
2	B	94	ASN	3.6
3	C	142	MET	3.6
6	F	4	TYR	3.6
8	H	30	ARG	3.6
2	B	215	LEU	3.6
4	D	19	LEU	3.6
4	D	135	LEU	3.6
5	E	129	ILE	3.5
19	S	66	MET	3.5
16	P	40	ASP	3.5
5	E	32	VAL	3.5
3	C	201	TYR	3.5
10	J	62	HIS	3.5
22	Y	3	MET	3.5
9	I	17	VAL	3.5
19	S	10	PHE	3.5
9	I	112	LYS	3.5
4	D	48	ALA	3.5
8	H	58	TYR	3.5
2	B	11	LEU	3.5
1	A	1368	G	3.4
9	I	102	LEU	3.4
19	S	71	LEU	3.4
1	A	1324	A	3.4
5	E	105	VAL	3.4
15	O	63	ARG	3.4
19	S	36	ARG	3.4
9	I	76	ALA	3.4
9	I	111	ARG	3.4
1	A	1040	U	3.4
6	F	65	VAL	3.4
2	B	152	PHE	3.4
13	M	68	GLY	3.4
9	I	116	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
13	M	8	GLU	3.4
13	M	23	TYR	3.4
14	N	23	ARG	3.4
10	J	98	ILE	3.4
9	I	118	LYS	3.4
12	L	69	TYR	3.4
18	R	55	ARG	3.4
1	A	1190	G	3.4
1	A	1257	U	3.4
1	A	1322	C	3.4
3	C	28	GLN	3.3
4	D	204	ILE	3.3
2	B	238	LEU	3.3
1	A	1315	U	3.3
1	A	981	U	3.3
2	B	69	LEU	3.3
10	J	70	ARG	3.3
18	R	85	LEU	3.3
3	C	35	GLU	3.3
12	L	14	GLY	3.3
7	G	28	ASN	3.3
20	T	40	ALA	3.3
1	A	853	G	3.3
13	M	82	MET	3.3
13	M	5	ALA	3.3
20	T	13	LEU	3.3
1	A	1108	G	3.3
4	D	114	ARG	3.3
9	I	64	THR	3.3
10	J	45	ARG	3.3
7	G	70	LYS	3.3
14	N	58	LYS	3.3
7	G	42	ILE	3.3
3	C	2	GLY	3.3
21	U	3	LYS	3.3
7	G	9	VAL	3.2
3	C	113	ALA	3.2
10	J	20	ALA	3.2
16	P	48	TRP	3.2
3	C	131	ARG	3.2
11	K	119	CYS	3.2
22	Y	42	SER	3.2

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Mol	Chain	Res	Type	RSRZ
16	P	9	PHE	3.2
13	M	100	GLY	3.2
4	D	68	TYR	3.2
18	R	45	SER	3.2
20	T	14	LYS	3.2
16	P	34	GLU	3.2
8	H	65	TYR	3.2
16	P	50	LYS	3.2
11	K	97	ALA	3.2
21	U	12	LYS	3.2
20	T	75	ASN	3.2
2	B	240	GLN	3.2
7	G	41	ARG	3.2
17	Q	35	VAL	3.1
19	S	81	ARG	3.1
2	B	7	VAL	3.1
2	B	184	VAL	3.1
10	J	44	VAL	3.1
22	Y	85	LEU	3.1
8	H	28	ALA	3.1
1	A	978	A	3.1
12	L	89	ARG	3.1
18	R	40	LEU	3.1
5	E	23	GLY	3.1
21	U	2	GLY	3.1
5	E	11	ILE	3.1
16	P	47	ASP	3.1
9	I	125	TYR	3.1
7	G	8	GLU	3.1
13	M	102	ARG	3.1
2	B	208	ILE	3.1
8	H	67	PRO	3.0
10	J	61	GLU	3.0
22	Y	45	PRO	3.0
8	H	54	ASP	3.0
22	Y	78	ILE	3.0
12	L	43	VAL	3.0
13	M	74	VAL	3.0
20	T	32	ALA	3.0
8	H	4	ASP	3.0
12	L	90	VAL	3.0
21	U	8	THR	3.0

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Mol	Chain	Res	Type	RSRZ
22	Y	33	HIS	3.0
7	G	72	ARG	3.0
17	Q	59	ILE	3.0
4	D	6	GLY	3.0
1	A	1045	C	3.0
13	M	25	ILE	3.0
16	P	13	HIS	3.0
3	C	31	HIS	3.0
11	K	50	TYR	3.0
1	A	1400	C	3.0
5	E	8	GLU	2.9
13	M	4	ILE	2.9
3	C	53	ALA	2.9
4	D	184	LYS	2.9
15	O	72	ARG	2.9
4	D	11	LEU	2.9
16	P	41	PRO	2.9
1	A	422	C	2.9
3	C	79	ARG	2.9
13	M	9	ILE	2.9
22	Y	32	THR	2.9
13	M	24	GLY	2.9
1	A	1394	A	2.9
5	E	125	SER	2.9
21	U	10	ARG	2.9
9	I	34	ASN	2.9
2	B	143	GLU	2.9
20	T	10	LEU	2.9
22	Y	27	LEU	2.9
19	S	69	HIS	2.9
4	D	197	PRO	2.9
12	L	27	LEU	2.9
19	S	48	THR	2.9
7	G	95	ARG	2.9
4	D	64	LEU	2.9
7	G	32	ARG	2.9
1	A	1249	C	2.9
7	G	96	GLN	2.9
20	T	99	LEU	2.8
17	Q	47	PRO	2.8
2	B	76	GLN	2.8
9	I	26	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
5	E	10	MET	2.8
13	M	70	LEU	2.8
21	U	17	THR	2.8
14	N	55	GLY	2.8
22	Y	46	GLN	2.8
18	R	86	VAL	2.8
4	D	43	HIS	2.8
4	D	70	ILE	2.8
7	G	27	ILE	2.8
10	J	33	GLN	2.8
1	A	852	G	2.8
12	L	41	ARG	2.8
4	D	146	ILE	2.8
8	H	93	VAL	2.8
2	B	132	LYS	2.8
6	F	36	ARG	2.8
11	K	60	ALA	2.8
22	Y	15	ALA	2.8
2	B	155	LEU	2.8
11	K	98	LEU	2.8
19	S	52	TYR	2.7
1	A	1356	G	2.7
8	H	108	GLY	2.7
1	A	1318	A	2.7
9	I	79	LEU	2.7
11	K	122	LYS	2.7
22	Y	89	GLN	2.7
3	C	198	VAL	2.7
2	B	164	VAL	2.7
13	M	75	ALA	2.7
3	C	54	ARG	2.7
1	A	970	C	2.7
22	Y	4	ASN	2.7
1	A	1186	G	2.7
9	I	69	GLY	2.7
15	O	40	SER	2.7
2	B	170	GLU	2.7
21	U	4	GLY	2.7
1	A	1320	C	2.7
10	J	58	ASP	2.7
19	S	65	ASN	2.7
2	B	81	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	180	LEU	2.6
2	B	112	VAL	2.6
18	R	42	ARG	2.6
22	Y	34	LEU	2.6
1	A	1014	A	2.6
3	C	26	LYS	2.6
14	N	11	LYS	2.6
1	A	961	U	2.6
8	H	32	LYS	2.6
3	C	55	VAL	2.6
7	G	113	GLU	2.6
12	L	66	VAL	2.6
14	N	50	LYS	2.6
2	B	163	PHE	2.6
4	D	65	ARG	2.6
16	P	22	THR	2.6
2	B	138	LEU	2.6
4	D	29	PRO	2.6
16	P	14	ASN	2.6
5	E	45	PHE	2.6
2	B	58	ILE	2.6
3	C	189	ALA	2.6
9	I	13	ALA	2.6
10	J	85	LEU	2.6
13	M	53	VAL	2.6
10	J	60	ARG	2.5
2	B	17	PHE	2.5
10	J	92	THR	2.5
9	I	108	VAL	2.5
2	B	209	ARG	2.5
1	A	617	G	2.5
1	A	1357	A	2.5
4	D	136	PRO	2.5
7	G	71	PRO	2.5
1	A	135	C	2.5
2	B	236	TYR	2.5
16	P	12	LYS	2.5
16	P	33	ILE	2.5
3	C	130	VAL	2.5
12	L	58	VAL	2.5
2	B	95	GLN	2.5
1	A	1285	A	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1317	C	2.5
16	P	51	VAL	2.5
21	U	9	ARG	2.5
10	J	6	ILE	2.5
1	A	200	G	2.5
1	A	854	G	2.5
20	T	8	ARG	2.5
12	L	46	LYS	2.5
14	N	42	ILE	2.5
1	A	1377	A	2.5
1	A	230	G	2.5
9	I	100	GLY	2.5
16	P	60	LEU	2.5
11	K	54	ARG	2.5
1	A	1007	C	2.5
3	C	153	VAL	2.5
5	E	72	GLN	2.5
10	J	72	VAL	2.5
1	A	630	G	2.4
8	H	1	MET	2.4
2	B	75	LYS	2.4
9	I	37	PHE	2.4
2	B	90	MET	2.4
15	O	47	LYS	2.4
20	T	34	LYS	2.4
1	A	1352	C	2.4
2	B	206	ASP	2.4
7	G	35	LYS	2.4
8	H	109	ILE	2.4
1	A	1360	A	2.4
1	A	966	G	2.4
15	O	46	HIS	2.4
3	C	37	GLN	2.4
5	E	123	LEU	2.4
8	H	136	GLU	2.4
22	Y	64	SER	2.4
4	D	103	ASN	2.4
10	J	96	ILE	2.4
5	E	73	ASN	2.4
1	A	1017	G	2.4
1	A	1258	G	2.4
1	A	1371	G	2.4

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Mol	Chain	Res	Type	RSRZ
5	E	13	ILE	2.4
7	G	16	LEU	2.4
10	J	35	SER	2.4
2	B	34	ALA	2.4
13	M	81	LEU	2.4
16	P	64	ALA	2.3
13	M	29	ARG	2.3
1	A	1118	C	2.3
16	P	67	THR	2.3
9	I	117	HIS	2.3
3	C	11	ARG	2.3
10	J	64	GLU	2.3
13	M	95	GLY	2.3
17	Q	69	LYS	2.3
14	N	59	ALA	2.3
15	O	36	ILE	2.3
1	A	1234	C	2.3
22	Y	67	HIS	2.3
14	N	35	ARG	2.3
4	D	63	LYS	2.3
20	T	63	ILE	2.3
1	A	993	G	2.3
1	A	1064	G	2.3
15	O	78	TYR	2.3
13	M	76	ALA	2.3
15	O	60	VAL	2.3
1	A	1250	A	2.3
1	A	1361	G	2.3
1	A	1359	C	2.3
20	T	73	HIS	2.3
20	T	70	SER	2.3
4	D	178	VAL	2.3
11	K	88	GLY	2.3
10	J	56	HIS	2.2
8	H	27	PRO	2.2
1	A	1230	C	2.2
1	A	1316	G	2.2
14	N	29	ARG	2.2
22	Y	95	ARG	2.2
15	O	80	ALA	2.2
3	C	13	GLY	2.2
10	J	36	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
13	M	38	GLY	2.2
15	O	59	MET	2.2
2	B	229	VAL	2.2
1	A	203	U	2.2
19	S	8	GLY	2.2
17	Q	48	GLU	2.2
3	C	17	ASP	2.2
3	C	149	ALA	2.2
7	G	25	ALA	2.2
1	A	1259	C	2.2
1	A	1020	U	2.2
5	E	106	PRO	2.2
9	I	123	PRO	2.2
10	J	83	GLU	2.2
3	C	27	LYS	2.2
1	A	1363(A)	A	2.2
2	B	39	ILE	2.2
5	E	145	LYS	2.2
15	O	34	LEU	2.2
22	Y	81	LEU	2.2
9	I	46	ALA	2.2
10	J	73	ASP	2.2
14	N	6	LEU	2.2
1	A	1369	C	2.2
6	F	1	MET	2.2
20	T	81	LYS	2.2
2	B	72	GLY	2.2
1	A	1042	G	2.2
16	P	36	ILE	2.2
9	I	16	ARG	2.2
17	Q	67	LYS	2.2
5	E	127	ASN	2.1
3	C	71	ALA	2.1
7	G	108	ALA	2.1
16	P	80	PHE	2.1
18	R	29	PHE	2.1
14	N	39	LEU	2.1
11	K	45	GLY	2.1
22	Y	59	GLY	2.1
3	C	64	VAL	2.1
16	P	21	VAL	2.1
17	Q	92	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
14	N	13	THR	2.1
20	T	65	LYS	2.1
4	D	102	ASP	2.1
1	A	841	U	2.1
4	D	21	LEU	2.1
3	C	78	GLY	2.1
11	K	86	GLY	2.1
1	A	1093	A	2.1
1	A	1362	C	2.1
2	B	8	LYS	2.1
7	G	104	LEU	2.1
16	P	16	HIS	2.1
1	A	976	G	2.1
2	B	88	ALA	2.1
12	L	51	ALA	2.1
9	I	14	VAL	2.1
3	C	8	ILE	2.1
10	J	50	ILE	2.1
14	N	34	TYR	2.1
8	H	90	GLY	2.1
12	L	88	GLY	2.1
16	P	8	ARG	2.1
7	G	127	ALA	2.1
12	L	94	PRO	2.1
1	A	951	G	2.1
8	H	63	LEU	2.1
16	P	10	GLY	2.1
1	A	936	C	2.0
20	T	80	ARG	2.0
19	S	73	GLU	2.0
1	A	1378	C	2.0
9	I	65	VAL	2.0
2	B	118	LEU	2.0
6	F	75	LEU	2.0
8	H	36	LEU	2.0
4	D	118	ARG	2.0
3	C	80	GLY	2.0
10	J	38	ILE	2.0
15	O	82	ILE	2.0
1	A	1262	C	2.0
1	A	1344	C	2.0
8	H	62	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
16	P	49	LEU	2.0
19	S	78	ARG	2.0
5	E	128	PRO	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	1713	1/1	0.08	-	55,55,55,55	0
23	MG	A	1725	1/1	0.09	-	60,60,60,60	0
23	MG	A	1675	1/1	0.19	-	80,80,80,80	0
23	MG	A	1735	1/1	0.13	-	79,79,79,79	0
23	MG	A	1694	1/1	0.09	-	73,73,73,73	0
23	MG	A	1601	1/1	0.17	-	55,55,55,55	0
23	MG	A	1654	1/1	0.43	-	85,85,85,85	0
23	MG	A	1678	1/1	0.23	-	86,86,86,86	0
23	MG	A	1727	1/1	0.16	-	77,77,77,77	0
23	MG	A	1800	1/1	0.16	-	67,67,67,67	0
23	MG	A	1711	1/1	0.24	-	55,55,55,55	0
23	MG	A	1693	1/1	0.05	-	64,64,64,64	0
23	MG	A	1750	1/1	0.28	-	69,69,69,69	0
23	MG	A	1720	1/1	0.36	-	90,90,90,90	0
23	MG	A	1704	1/1	0.10	-	46,46,46,46	0
23	MG	A	1787	1/1	0.37	-	84,84,84,84	0
23	MG	A	1614	1/1	0.29	-	70,70,70,70	0
23	MG	A	1783	1/1	0.11	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1687	1/1	0.10	-	67,67,67,67	0
23	MG	A	1802	1/1	0.18	-	76,76,76,76	0
23	MG	A	1631	1/1	0.23	-	87,87,87,87	0
23	MG	E	201	1/1	0.14	-	78,78,78,78	0
23	MG	A	1778	1/1	0.18	-	130,130,130,130	0
23	MG	A	1625	1/1	0.30	-	69,69,69,69	0
23	MG	A	1663	1/1	0.16	-	54,54,54,54	0
23	MG	A	1728	1/1	0.42	-	63,63,63,63	0
23	MG	A	1744	1/1	0.15	-	65,65,65,65	0
23	MG	A	1703	1/1	0.28	-	55,55,55,55	0
24	ZN	D	301	1/1	0.15	-	93,93,93,93	0
23	MG	A	1611	1/1	0.31	-	56,56,56,56	0
23	MG	A	1791	1/1	0.09	-	66,66,66,66	0
23	MG	A	1700	1/1	0.16	-	73,73,73,73	0
23	MG	A	1718	1/1	0.12	-	85,85,85,85	0
23	MG	A	1605	1/1	0.35	-	63,63,63,63	0
23	MG	A	1751	1/1	0.15	-	88,88,88,88	0
23	MG	A	1661	1/1	0.14	-	65,65,65,65	0
23	MG	A	1685	1/1	0.23	-	82,82,82,82	0
23	MG	A	1755	1/1	0.20	-	77,77,77,77	0
23	MG	A	1796	1/1	0.10	-	57,57,57,57	0
23	MG	A	1730	1/1	0.19	-	84,84,84,84	0
23	MG	A	1617	1/1	0.21	-	63,63,63,63	0
23	MG	A	1619	1/1	0.16	-	56,56,56,56	0
23	MG	A	1621	1/1	0.21	-	87,87,87,87	0
23	MG	A	1759	1/1	0.09	-	64,64,64,64	0
23	MG	A	1762	1/1	0.14	-	92,92,92,92	0
23	MG	A	1771	1/1	0.21	-	71,71,71,71	0
23	MG	A	1629	1/1	0.20	-	81,81,81,81	0
23	MG	A	1752	1/1	0.18	-	89,89,89,89	0
23	MG	A	1788	1/1	0.21	-	83,83,83,83	0
23	MG	A	1716	1/1	0.73	-	85,85,85,85	0
23	MG	A	1644	1/1	0.15	-	63,63,63,63	0
23	MG	A	1604	1/1	0.46	-	70,70,70,70	0
23	MG	A	1681	1/1	0.26	-	92,92,92,92	0
23	MG	A	1651	1/1	0.10	-	65,65,65,65	0
23	MG	A	1773	1/1	0.28	-	61,61,61,61	0
23	MG	A	1792	1/1	0.28	-	48,48,48,48	0
24	ZN	N	101	1/1	0.06	-	108,108,108,108	0
23	MG	A	1674	1/1	0.22	-	73,73,73,73	0
23	MG	A	1633	1/1	0.36	-	50,50,50,50	0
23	MG	A	1795	1/1	0.10	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1775	1/1	0.20	-	73,73,73,73	0
23	MG	A	1769	1/1	0.28	-	95,95,95,95	0
23	MG	A	1756	1/1	0.15	-	79,79,79,79	0
23	MG	A	1691	1/1	0.12	-	75,75,75,75	0
23	MG	A	1729	1/1	0.19	-	79,79,79,79	0
23	MG	A	1672	1/1	0.18	-	78,78,78,78	0
23	MG	A	1807	1/1	0.10	-	61,61,61,61	0
23	MG	A	1692	1/1	0.21	-	74,74,74,74	0
23	MG	A	1806	1/1	0.28	-	38,38,38,38	0
23	MG	A	1665	1/1	0.12	-	62,62,62,62	0
23	MG	A	1709	1/1	0.28	-	73,73,73,73	0
23	MG	A	1624	1/1	0.26	-	65,65,65,65	0
23	MG	A	1777	1/1	0.10	-	76,76,76,76	0
23	MG	A	1798	1/1	0.11	-	85,85,85,85	0
23	MG	A	1803	1/1	0.15	-	88,88,88,88	0
23	MG	A	1733	1/1	0.12	-	63,63,63,63	0
23	MG	A	1662	1/1	0.26	-	55,55,55,55	0
23	MG	A	1723	1/1	0.11	-	58,58,58,58	0
23	MG	A	1626	1/1	0.51	-	86,86,86,86	0
23	MG	A	1695	1/1	0.14	-	69,69,69,69	0
23	MG	A	1712	1/1	0.15	-	55,55,55,55	0
23	MG	A	1655	1/1	0.62	-	63,63,63,63	0
23	MG	A	1613	1/1	0.27	-	68,68,68,68	0
23	MG	A	1696	1/1	0.16	-	76,76,76,76	0
23	MG	A	1664	1/1	0.24	-	75,75,75,75	0
23	MG	A	1643	1/1	0.10	-	76,76,76,76	0
23	MG	A	1766	1/1	0.11	-	87,87,87,87	0
23	MG	A	1799	1/1	0.18	-	68,68,68,68	0
23	MG	A	1804	1/1	0.11	-	60,60,60,60	0
23	MG	A	1786	1/1	0.26	-	53,53,53,53	0
23	MG	A	1731	1/1	0.10	-	65,65,65,65	0
23	MG	A	1736	1/1	0.99	-	85,85,85,85	0
23	MG	A	1609	1/1	0.37	-	77,77,77,77	0
23	MG	A	1666	1/1	0.08	-	60,60,60,60	0
23	MG	A	1668	1/1	0.22	-	66,66,66,66	0
23	MG	A	1764	1/1	0.08	-	66,66,66,66	0
23	MG	A	1748	1/1	0.38	-	63,63,63,63	0
23	MG	Q	201	1/1	0.12	-	76,76,76,76	0
23	MG	A	1639	1/1	0.58	-	57,57,57,57	0
23	MG	A	1637	1/1	0.57	-	98,98,98,98	0
23	MG	A	1647	1/1	0.15	-	103,103,103,103	0
23	MG	A	1684	1/1	0.14	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1680	1/1	0.19	-	53,53,53,53	0
23	MG	A	1724	1/1	0.13	-	66,66,66,66	0
23	MG	A	1790	1/1	0.29	-	51,51,51,51	0
23	MG	A	1784	1/1	0.13	-	63,63,63,63	0
23	MG	A	1770	1/1	0.11	-	58,58,58,58	0
23	MG	A	1793	1/1	0.09	-	72,72,72,72	0
23	MG	A	1701	1/1	0.11	-	56,56,56,56	0
23	MG	A	1660	1/1	0.10	-	89,89,89,89	0
23	MG	A	1677	1/1	0.16	-	64,64,64,64	0
23	MG	A	1618	1/1	0.21	-	61,61,61,61	0
23	MG	A	1656	1/1	0.16	-	66,66,66,66	0
23	MG	A	1757	1/1	0.21	-	77,77,77,77	0
23	MG	A	1710	1/1	0.22	-	76,76,76,76	0
23	MG	A	1721	1/1	0.31	-	84,84,84,84	0
23	MG	A	1602	1/1	0.88	-	70,70,70,70	0
23	MG	A	1779	1/1	0.17	-	60,60,60,60	0
23	MG	A	1658	1/1	0.23	-	85,85,85,85	0
23	MG	A	1726	1/1	0.15	-	91,91,91,91	0
23	MG	A	1698	1/1	0.08	-	95,95,95,95	0
23	MG	A	1739	1/1	0.12	-	52,52,52,52	0
23	MG	A	1738	1/1	0.18	-	75,75,75,75	0
23	MG	A	1760	1/1	0.07	-	95,95,95,95	0
23	MG	A	1768	1/1	0.17	-	86,86,86,86	0
23	MG	A	1642	1/1	1.02	-	64,64,64,64	0
23	MG	A	1607	1/1	0.30	-	96,96,96,96	0
23	MG	A	1697	1/1	0.08	-	71,71,71,71	0
23	MG	A	1627	1/1	0.55	-	72,72,72,72	0
23	MG	A	1719	1/1	0.14	-	76,76,76,76	0
23	MG	A	1767	1/1	0.15	-	65,65,65,65	0
23	MG	A	1640	1/1	0.58	-	63,63,63,63	0
23	MG	A	1780	1/1	0.15	-	83,83,83,83	0
23	MG	A	1758	1/1	0.07	-	75,75,75,75	0
23	MG	A	1774	1/1	0.17	-	89,89,89,89	0
23	MG	A	1673	1/1	0.09	-	74,74,74,74	0
23	MG	A	1734	1/1	0.26	-	89,89,89,89	0
23	MG	A	1761	1/1	0.34	-	93,93,93,93	0
23	MG	A	1706	1/1	0.23	-	72,72,72,72	0
23	MG	A	1740	1/1	0.21	-	76,76,76,76	0
23	MG	A	1667	1/1	0.19	-	71,71,71,71	0
23	MG	A	1620	1/1	0.16	-	74,74,74,74	0
23	MG	A	1623	1/1	0.46	-	60,60,60,60	0
23	MG	A	1615	1/1	0.14	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1688	1/1	0.17	-	68,68,68,68	0
23	MG	A	1649	1/1	0.14	-	67,67,67,67	0
23	MG	A	1686	1/1	0.13	-	62,62,62,62	0
23	MG	A	1616	1/1	0.42	-	71,71,71,71	0
23	MG	A	1742	1/1	0.18	-	117,117,117,117	0
23	MG	A	1650	1/1	0.38	-	67,67,67,67	0
23	MG	A	1714	1/1	0.62	-	95,95,95,95	0
23	MG	A	1702	1/1	0.16	-	74,74,74,74	0
23	MG	A	1749	1/1	0.16	-	57,57,57,57	0
23	MG	A	1610	1/1	0.85	-	67,67,67,67	0
23	MG	A	1634	1/1	0.08	-	40,40,40,40	0
23	MG	A	1657	1/1	0.16	-	66,66,66,66	0
23	MG	A	1690	1/1	0.14	-	90,90,90,90	0
23	MG	A	1682	1/1	0.17	-	83,83,83,83	0
23	MG	A	1608	1/1	0.22	-	54,54,54,54	0
23	MG	A	1765	1/1	0.11	-	90,90,90,90	0
23	MG	A	1648	1/1	0.17	-	72,72,72,72	0
23	MG	A	1754	1/1	0.13	-	74,74,74,74	0
23	MG	A	1636	1/1	0.17	-	58,58,58,58	0
23	MG	A	1670	1/1	0.12	-	71,71,71,71	0
23	MG	A	1776	1/1	0.31	-	78,78,78,78	0
23	MG	A	1782	1/1	0.48	-	74,74,74,74	0
23	MG	A	1630	1/1	0.31	-	78,78,78,78	0
23	MG	A	1628	1/1	0.29	-	71,71,71,71	0
23	MG	A	1653	1/1	0.14	-	88,88,88,88	0
23	MG	A	1612	1/1	0.77	-	84,84,84,84	0
23	MG	A	1708	1/1	0.13	-	73,73,73,73	0
23	MG	A	1789	1/1	0.28	-	84,84,84,84	0
23	MG	A	1746	1/1	0.29	-	52,52,52,52	0
23	MG	A	1785	1/1	0.38	-	73,73,73,73	0
23	MG	A	1707	1/1	0.34	-	76,76,76,76	0
23	MG	A	1632	1/1	0.85	-	57,57,57,57	0
23	MG	A	1679	1/1	0.13	-	55,55,55,55	0
23	MG	A	1641	1/1	0.50	-	62,62,62,62	0
23	MG	A	1763	1/1	0.56	-	86,86,86,86	0
23	MG	A	1741	1/1	0.28	-	72,72,72,72	0
23	MG	A	1669	1/1	0.08	-	65,65,65,65	0
23	MG	A	1722	1/1	0.08	-	53,53,53,53	0
23	MG	A	1797	1/1	0.04	-	66,66,66,66	0
23	MG	A	1705	1/1	0.16	-	71,71,71,71	0
23	MG	A	1659	1/1	0.07	-	64,64,64,64	0
23	MG	A	1699	1/1	0.43	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1747	1/1	0.41	-	113,113,113,113	0
23	MG	A	1801	1/1	0.11	-	99,99,99,99	0
23	MG	A	1781	1/1	0.26	-	116,116,116,116	0
23	MG	A	1689	1/1	0.45	-	110,110,110,110	0
23	MG	A	1646	1/1	0.09	-	71,71,71,71	0
23	MG	A	1645	1/1	0.85	-	69,69,69,69	0
23	MG	A	1732	1/1	0.15	-	62,62,62,62	0
23	MG	A	1745	1/1	0.09	-	69,69,69,69	0
23	MG	A	1683	1/1	0.12	-	60,60,60,60	0
23	MG	A	1638	1/1	0.51	-	65,65,65,65	0
23	MG	A	1676	1/1	0.26	-	75,75,75,75	0
23	MG	A	1772	1/1	0.41	-	71,71,71,71	0
23	MG	A	1805	1/1	0.13	-	55,55,55,55	0
23	MG	A	1737	1/1	0.21	-	94,94,94,94	0
23	MG	A	1717	1/1	0.19	-	49,49,49,49	0
23	MG	A	1794	1/1	0.10	-	65,65,65,65	0
23	MG	A	1603	1/1	0.49	-	83,83,83,83	0
23	MG	A	1671	1/1	0.13	-	80,80,80,80	0
23	MG	A	1635	1/1	0.22	-	63,63,63,63	0
23	MG	A	1622	1/1	0.34	-	65,65,65,65	0
23	MG	A	1743	1/1	0.10	-	99,99,99,99	0
23	MG	A	1715	1/1	0.14	-	67,67,67,67	0
23	MG	A	1753	1/1	0.10	-	91,91,91,91	0
23	MG	A	1652	1/1	0.40	-	55,55,55,55	0
23	MG	A	1808	1/1	0.32	-	45,45,45,45	0
23	MG	A	1606	1/1	0.45	-	83,83,83,83	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.