



Full wwPDB X-ray Structure Validation Report

Oct 10, 2014 – 02:28 PM EDT

PDB ID : 4RB7
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with amicoumacin, mRNA and three deacylated tRNAs in the A, P and E sites
Authors : Polikanov, Y.S.; Osterman, I.A.; Szal, T.; Tashlitsky, V.N.; Serebryakova, M.V.; Kusochev, P.; Bulkley, D.; Malanicheva, I.A.; Efimenko, T.A.; Efremenkova, O.V.; Konevega, A.L.; Shaw, K.J.; Bogdanov, A.A.; Rodnina, M.V.; Dontsova, O.A.; Mankin, A.S.; Steitz, T.A.; Sergiev, P.V.
Deposited on : 2014-09-12
Resolution : 2.40 Å(reported)

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

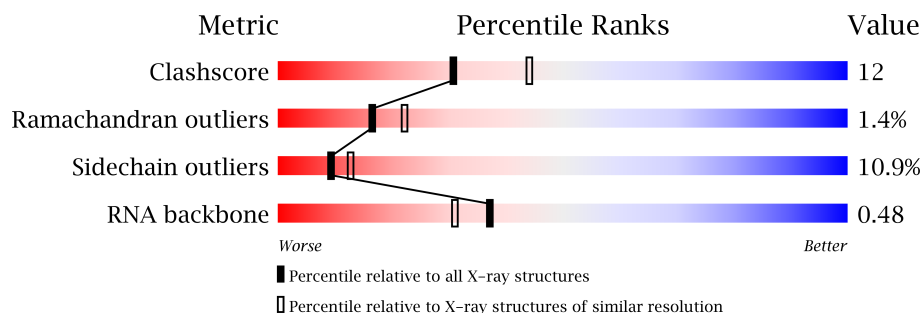
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23828

1 Overall quality at a glance

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RNA backbone	1838	1029 (3.00-1.80)







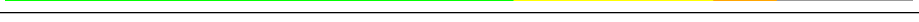

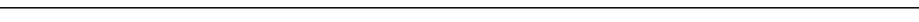


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1521	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	

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Mol	Chain	Length	Quality of chain
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	24	
23	W	76	
23	Y	76	
24	X	77	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 56383 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	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	231	Total	C	N	O	S	0	0	0
			1825	1167	326	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
			1542	968	300	273	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
			1674	1050	333	284	7			

- 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
			1133	716	214	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			816	516	146	151	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
			1235	769	244	216	6			

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			978	619	190	169			

- 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
			714	445	138	131			

- 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
			833	519	156	155	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
			930	585	185	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- 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
			492	312	104	72	4			

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			728	456	144	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
			677	430	133	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
			823	528	151	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	68	Total	C	N	O	0	0	0
			555	355	108	92			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

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

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 23 is a RNA chain called A/P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	W	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
23	Y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 24 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	X	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

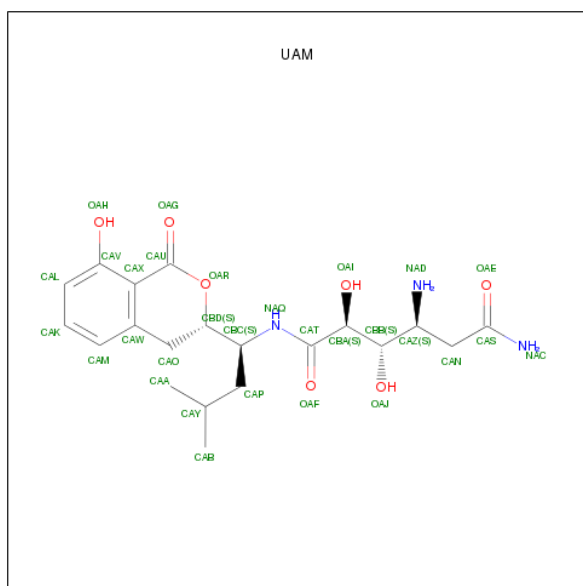
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	P	1	Total	Mg	0	0
			1	1		
25	G	1	Total	Mg	0	0
			1	1		
25	J	2	Total	Mg	0	0
			2	2		
25	Q	2	Total	Mg	0	0
			2	2		
25	D	2	Total	Mg	0	0
			2	2		
25	K	1	Total	Mg	0	0
			1	1		
25	E	1	Total	Mg	0	0
			1	1		
25	V	1	Total	Mg	0	0
			1	1		

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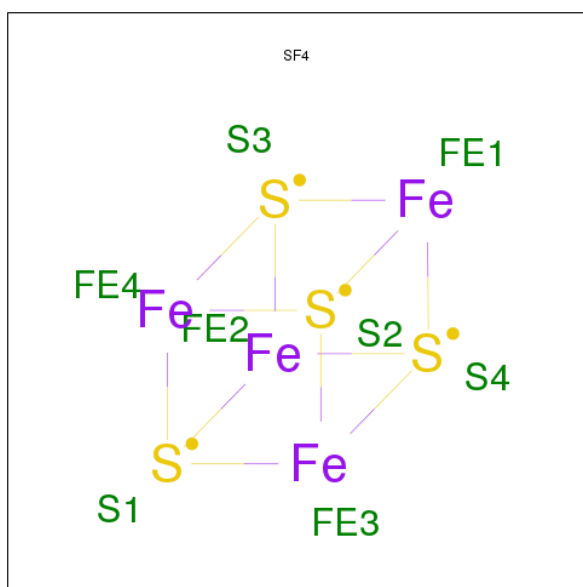
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	W	4	Total 4 Mg 4	0	0
25	A	201	Total 201 Mg 201	0	0
25	T	1	Total 1 Mg 1	0	0
25	X	6	Total 6 Mg 6	0	0
25	R	1	Total 1 Mg 1	0	0
25	L	2	Total 2 Mg 2	0	0
25	F	2	Total 2 Mg 2	0	0

- Molecule 26 is AMICOUMACIN A (three-letter code: UAM) (formula: $C_{20}H_{29}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			30	20	3	7		

- Molecule 27 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	N	1	Total	Zn	0	0
			1	1		

- Molecule 29 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	X	1	Total	K	0	0
			1	1		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	204	Total	O	0	0
			204	204		
30	D	1	Total	O	0	0
			1	1		
30	G	1	Total	O	0	0
			1	1		
30	I	1	Total	O	0	0
			1	1		

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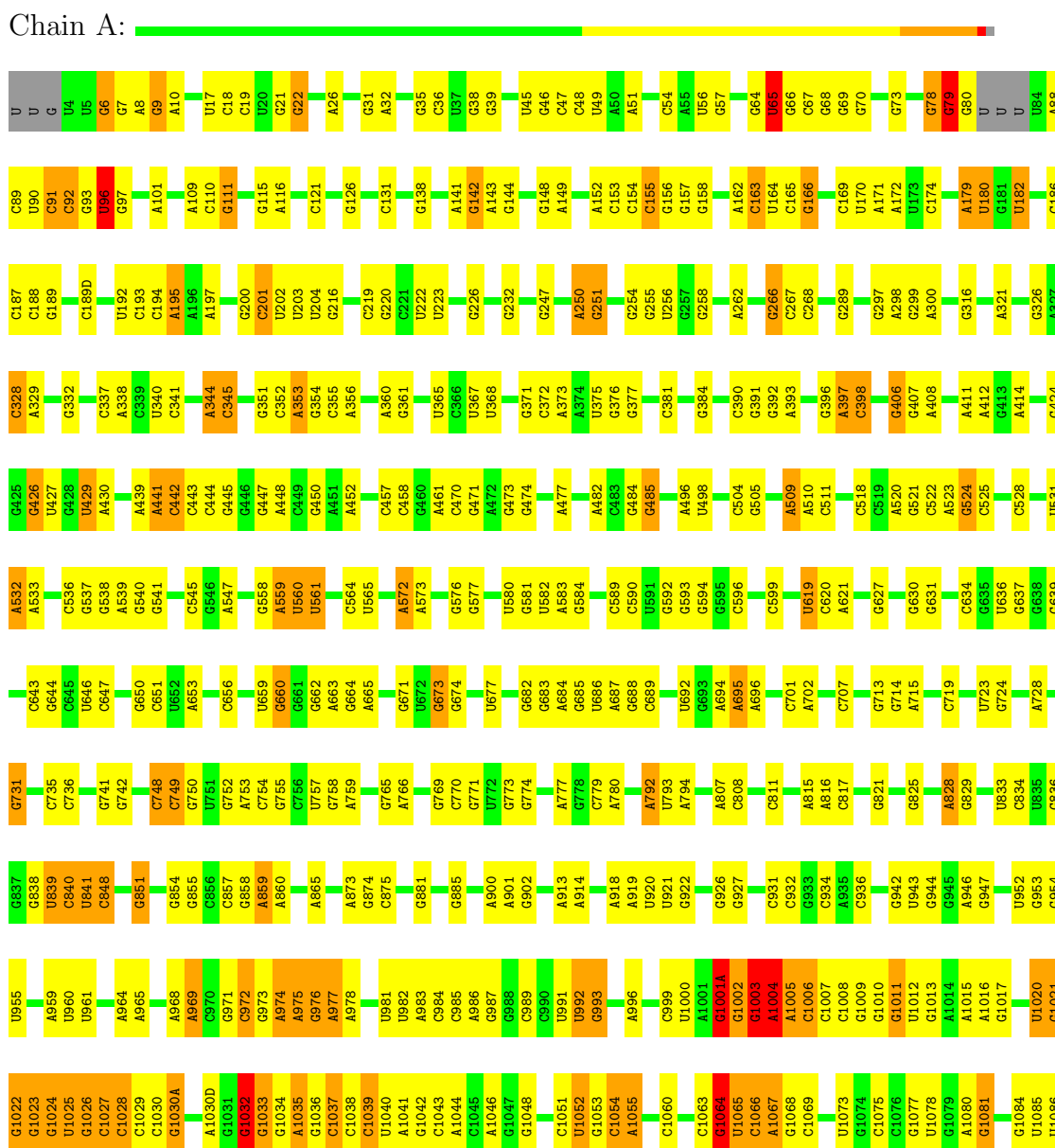
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	J	4	Total 4	O 4	0	0
30	L	4	Total 4	O 4	0	0
30	O	1	Total 1	O 1	0	0
30	P	1	Total 1	O 1	0	0
30	R	1	Total 1	O 1	0	0
30	T	1	Total 1	O 1	0	0
30	W	2	Total 2	O 2	0	0
30	X	6	Total 6	O 6	0	0

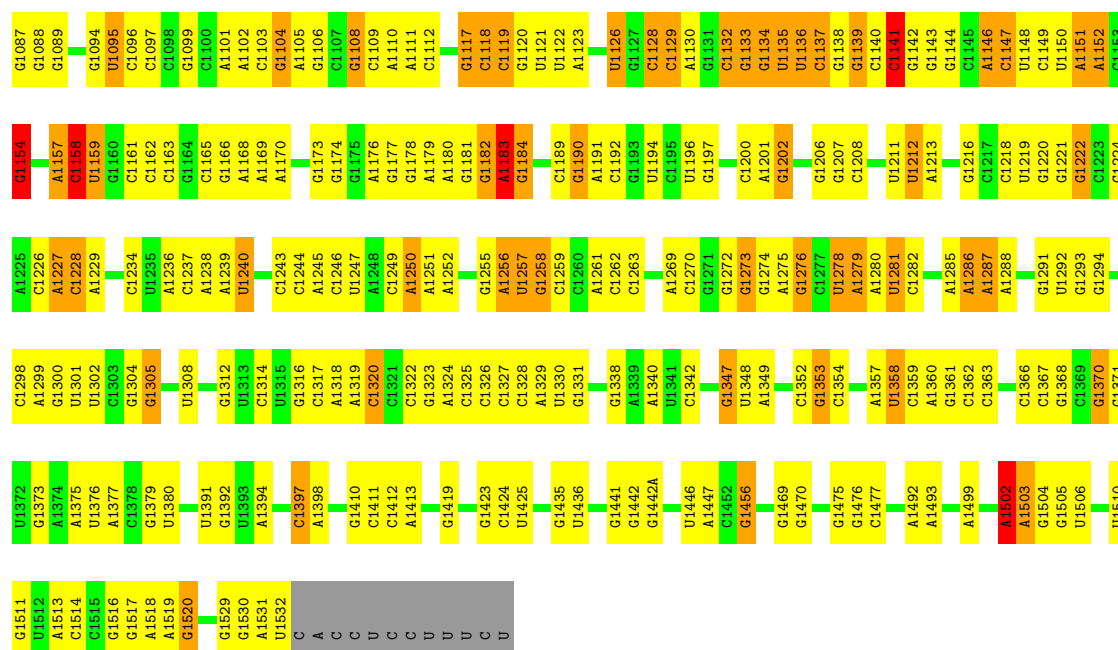
3 Residue-property plots

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

Note EDS was not executed.

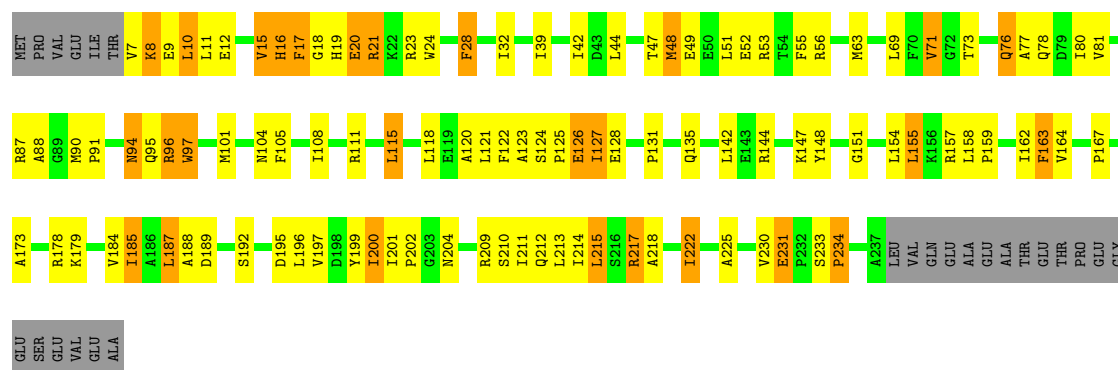
• Molecule 1: 16S Ribosomal RNA





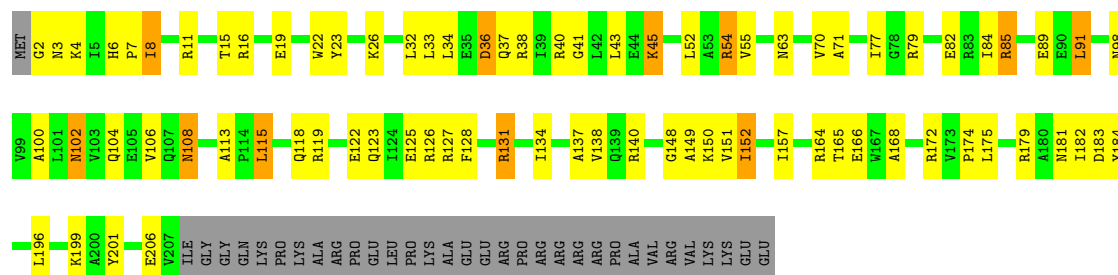
• Molecule 2: 30S Ribosomal Protein S2

Chain B:



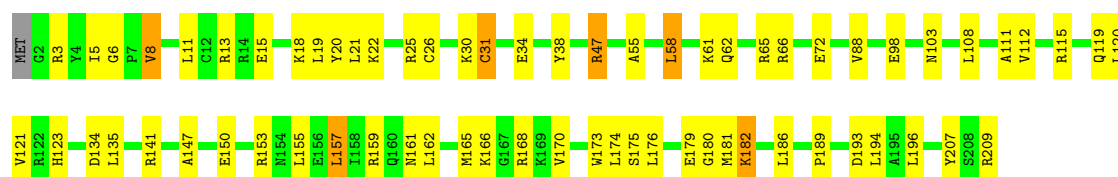
• Molecule 3: 30S Ribosomal Protein S3

Chain C:



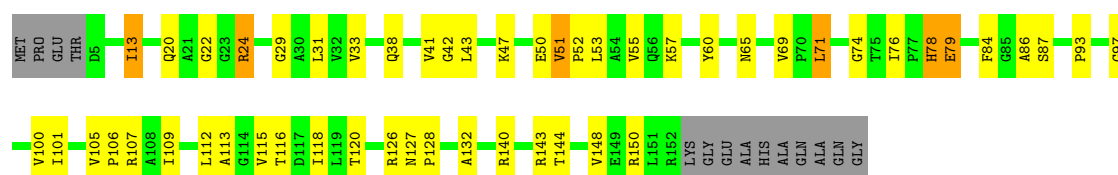
• Molecule 4: 30S Ribosomal Protein S4

Chain D:



• Molecule 5: 30S Ribosomal Protein S5

Chain E:



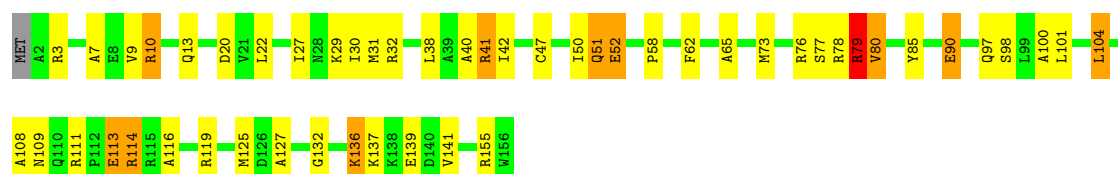
• Molecule 6: 30S Ribosomal Protein S6

Chain F:



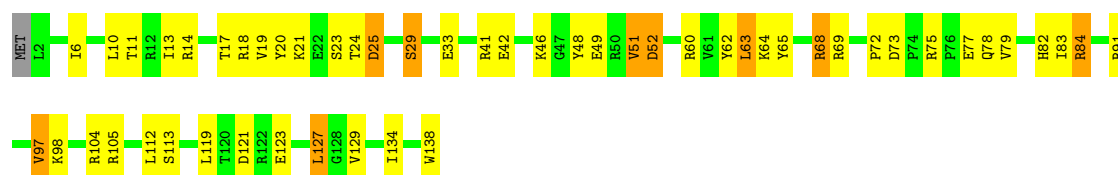
• Molecule 7: 30S Ribosomal Protein S7

Chain G:



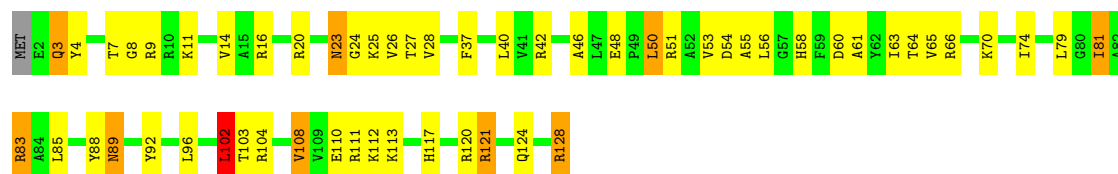
• Molecule 8: 30S Ribosomal Protein S8

Chain H:



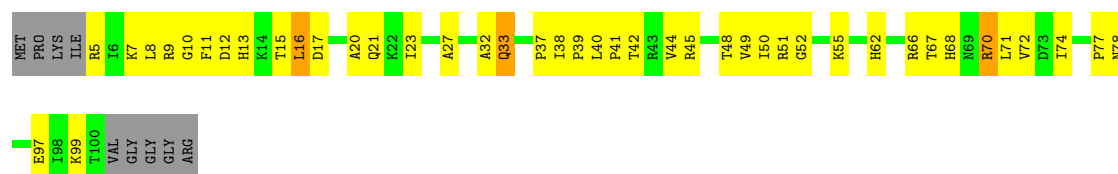
• Molecule 9: 30S Ribosomal Protein S9

Chain I:



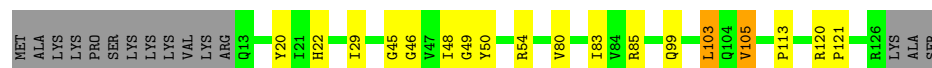
• Molecule 10: 30S Ribosomal Protein S10

Chain J: 



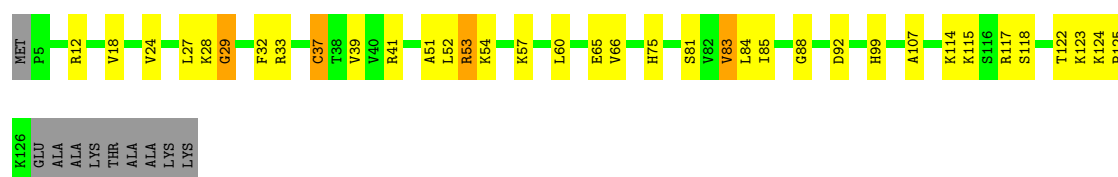
- Molecule 11: 30S Ribosomal Protein S11

Chain K: 



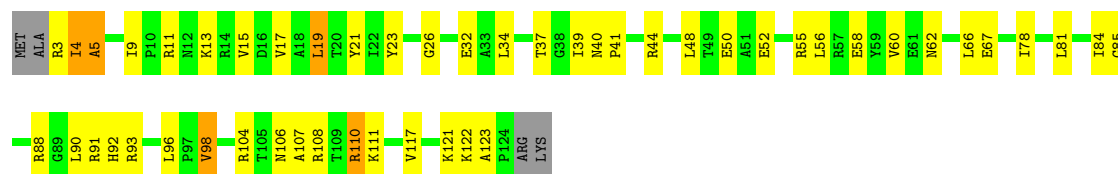
- Molecule 12: 30S Ribosomal Protein S12

Chain L: 



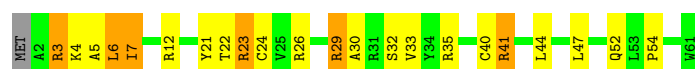
- Molecule 13: 30S Ribosomal Protein S13

Chain M: 



- Molecule 14: 30S Ribosomal Protein S14

Chain N: 



- Molecule 15: 30S Ribosomal Protein S15

Chain O: 



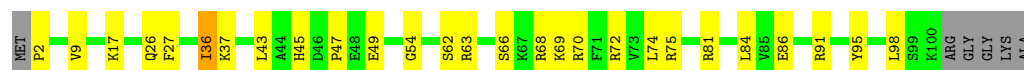
- Molecule 16: 30S Ribosomal Protein S16

Chain P: 



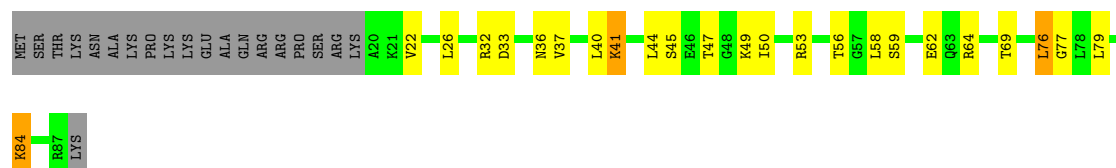
- Molecule 17: 30S Ribosomal Protein S17

Chain Q: 



- Molecule 18: 30S Ribosomal Protein S18

Chain R: 



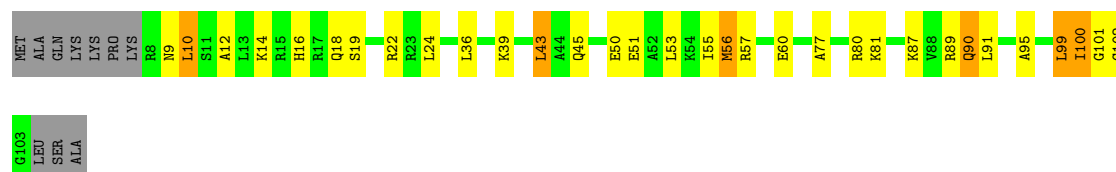
- Molecule 19: 30S Ribosomal Protein S19

Chain S: 



- Molecule 20: 30S Ribosomal Protein S20

Chain T: 



- Molecule 21: 30S Ribosomal Protein THX

Chain U: 



- Molecule 22: mRNA

Chain V: 



- Molecule 23: A/P-site tRNA

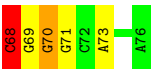
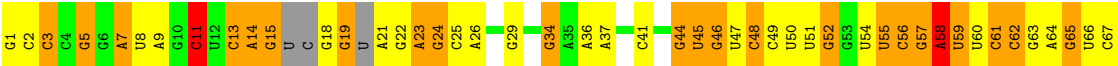
Chain W: 





• Molecule 23: A/P-site tRNA

Chain Y:



• Molecule 24: E-site tRNA

Chain X:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.06Å 448.57Å 623.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	256.12 – 2.40	Depositor
% Data completeness (in resolution range)	99.7 (256.12-2.40)	Depositor
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.237 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	56383	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, MIA, SF4, MG, UAM, 5MC, 4SU, 7MG, K, PSU

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	0.37	1/36170 (0.0%)	0.91	47/56452 (0.1%)
2	B	0.30	0/1860	0.61	1/2518 (0.0%)
3	C	0.30	0/1566	0.56	0/2119
4	D	0.29	0/1704	0.50	0/2284
5	E	0.31	0/1149	0.57	0/1548
6	F	0.30	0/829	0.51	0/1123
7	G	0.27	0/1254	0.53	0/1683
8	H	0.27	0/1108	0.49	0/1494
9	I	0.28	0/997	0.53	1/1343 (0.1%)
10	J	0.29	0/727	0.55	0/988
11	K	0.28	0/848	0.51	0/1149
12	L	0.29	0/946	0.56	1/1274 (0.1%)
13	M	0.28	0/961	0.55	0/1291
14	N	0.30	0/501	0.55	0/664
15	O	0.29	0/739	0.52	0/985
16	P	0.28	0/693	0.50	0/935
17	Q	0.27	0/836	0.48	0/1117
18	R	0.26	0/560	0.49	0/746
19	S	0.31	0/661	0.64	0/893
20	T	0.28	0/729	0.52	0/965
21	U	0.30	0/203	0.51	0/266
22	V	0.40	0/310	0.89	1/480 (0.2%)
23	W	0.51	0/1556	1.23	9/2418 (0.4%)
23	Y	0.56	1/1583 (0.1%)	1.22	12/2459 (0.5%)
24	X	0.49	0/1725	1.13	14/2689 (0.5%)
All	All	0.36	2/60215 (0.0%)	0.85	86/89883 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	1	G	OP3-P	-10.36	1.48	1.61
1	A	1154	G	C6-N1	-5.24	1.35	1.39

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1154	G	C5-C6-O6	12.79	136.28	128.60
24	X	46	G	C6-N1-C2	-9.19	119.59	125.10
1	A	1004	A	O4'-C1'-N9	8.95	115.36	108.20
1	A	1119	C	C2-N3-C4	8.93	124.36	119.90
1	A	1001(A)	G	N3-C4-N9	8.73	131.24	126.00
1	A	1154	G	N1-C6-O6	-8.44	114.84	119.90
24	X	14	A	C4-C5-C6	8.25	121.13	117.00
1	A	1001(A)	G	C8-N9-C1'	-7.80	116.85	127.00
1	A	1001(A)	G	C4-N9-C1'	7.67	136.47	126.50
1	A	79	G	C5-C6-O6	7.41	133.04	128.60
1	A	1119	C	C5-C4-N4	7.24	125.27	120.20
24	X	14	A	C5-N7-C8	7.20	107.50	103.90
1	A	754	C	C2-N1-C1'	7.16	126.68	118.80
1	A	1119	C	N3-C4-C5	-7.16	119.04	121.90
1	A	96	U	O4'-C1'-N1	6.89	113.71	108.20
1	A	1003	G	C4-N9-C1'	6.81	135.35	126.50
23	W	50	U	C5-C4-O4	-6.70	121.88	125.90
1	A	1183	A	P-O3'-C3'	6.67	127.71	119.70
24	X	14	A	C5-C6-N1	-6.59	114.41	117.70
23	Y	22	G	C8-N9-C1'	-6.52	118.53	127.00
23	Y	22	G	C4-N9-C1'	6.51	134.96	126.50
1	A	1003	G	N7-C8-N9	6.50	116.35	113.10
1	A	754	C	N1-C2-O2	6.45	122.77	118.90
24	X	22	G	N1-C6-O6	-6.40	116.06	119.90
1	A	1020	U	N1-C2-O2	6.39	127.27	122.80
23	W	25	C	C6-N1-C2	-6.36	117.76	120.30
24	X	46	G	C5-C6-N1	6.34	114.67	111.50
23	Y	11	C	C5-C6-N1	6.32	124.16	121.00
1	A	1001(A)	G	N9-C4-C5	-6.26	102.90	105.40
1	A	1064	G	P-O3'-C3'	6.08	127.00	119.70
24	X	14	A	C4-N9-C1'	6.01	137.11	126.30
1	A	792	A	O4'-C1'-N9	5.96	112.97	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	22	G	C5-N7-C8	-5.90	101.35	104.30
1	A	1001(A)	G	C6-C5-N7	-5.89	126.86	130.40
24	X	14	A	C8-N9-C1'	-5.85	117.17	127.70
1	A	1286	A	N7-C8-N9	5.84	116.72	113.80
1	A	1158	C	N1-C2-O2	5.83	122.40	118.90
1	A	1154	G	C6-N1-C2	5.83	128.59	125.10
24	X	22	G	C4-C5-C6	-5.80	115.32	118.80
23	Y	11	C	C2-N1-C1'	5.79	125.17	118.80
1	A	1126	U	C2-N1-C1'	5.77	124.62	117.70
1	A	1023	G	N3-C4-N9	5.73	129.44	126.00
1	A	1020	U	N3-C2-O2	-5.71	118.20	122.20
23	W	71	G	N3-C4-N9	5.70	129.42	126.00
1	A	1158	C	C2-N1-C1'	5.68	125.05	118.80
23	Y	11	C	C2-N3-C4	5.65	122.73	119.90
24	X	17	C	C2-N1-C1'	5.60	124.96	118.80
1	A	754	C	C6-N1-C1'	-5.59	114.09	120.80
23	W	71	G	C8-N9-C1'	-5.56	119.77	127.00
1	A	1032	G	N3-C4-N9	-5.53	122.68	126.00
1	A	1183	A	OP1-P-O3'	5.53	117.36	105.20
1	A	1154	G	N3-C2-N2	5.52	123.77	119.90
23	Y	7	A	O5'-P-OP2	-5.50	100.75	105.70
1	A	1001(A)	G	N3-C4-C5	-5.49	125.85	128.60
1	A	1154	G	N1-C2-N2	-5.48	111.27	116.20
23	Y	5	G	C5-C6-O6	-5.48	125.31	128.60
1	A	1286	A	C8-N9-C4	-5.48	103.61	105.80
1	A	79	G	N1-C6-O6	-5.47	116.62	119.90
23	Y	22	G	N3-C4-N9	5.46	129.28	126.00
1	A	1502	A	N1-C2-N3	5.46	132.03	129.30
1	A	1003	G	N3-C4-N9	5.44	129.26	126.00
1	A	1141	C	C2-N1-C1'	-5.38	112.88	118.80
23	Y	11	C	N1-C2-O2	5.38	122.13	118.90
24	X	20	U	C2-N1-C1'	5.38	124.16	117.70
1	A	1032	G	C5-C6-O6	5.37	131.82	128.60
23	Y	68	C	N1-C2-O2	5.35	122.11	118.90
9	I	102	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	1003	G	C8-N9-C1'	-5.29	120.12	127.00
1	A	1133	G	N3-C4-N9	-5.29	122.83	126.00
23	W	36	A	C6-N1-C2	5.26	121.76	118.60
23	W	3	C	C5-C6-N1	5.26	123.63	121.00
24	X	22	G	C5-C6-N1	5.25	114.13	111.50
1	A	65	U	P-O3'-C3'	5.24	125.99	119.70
1	A	1154	G	C5-C6-N1	-5.24	108.88	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	25	C	O4'-C1'-N1	5.22	112.37	108.20
1	A	1141	C	C6-N1-C1'	5.22	127.06	120.80
23	W	71	G	C4-N9-C1'	5.19	133.25	126.50
12	L	29	GLY	N-CA-C	-5.18	100.16	113.10
23	W	50	U	N3-C4-O4	5.15	123.01	119.40
22	V	19	U	C5-C4-O4	5.13	128.98	125.90
1	A	1133	G	N9-C4-C5	5.12	107.45	105.40
24	X	20	U	N1-C2-O2	5.11	126.37	122.80
1	A	1032	G	C6-C5-N7	5.08	133.45	130.40
23	Y	68	C	C2-N1-C1'	5.06	124.37	118.80
23	Y	58	A	OP1-P-O3'	5.05	116.32	105.20
2	B	115	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	79	ARG	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	32312	0	16307	511	0
2	B	1825	0	1828	83	0
3	C	1542	0	1517	55	0
4	D	1674	0	1714	43	0
5	E	1133	0	1191	38	0
6	F	816	0	808	11	0
7	G	1235	0	1249	32	0
8	H	1088	0	1126	39	0
9	I	978	0	966	46	0
10	J	714	0	672	36	0
11	K	833	0	836	10	0
12	L	930	0	980	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	950	0	988	34	0
14	N	492	0	529	17	0
15	O	728	0	760	23	0
16	P	677	0	686	18	0
17	Q	823	0	891	14	0
18	R	555	0	618	17	0
19	S	646	0	644	29	0
20	T	727	0	796	21	0
21	U	199	0	208	5	0
22	V	277	0	140	6	0
23	W	1544	0	788	38	0
23	Y	1565	0	795	61	0
24	X	1625	0	828	17	0
25	A	201	0	0	0	0
25	D	2	0	0	0	0
25	E	1	0	0	0	0
25	F	2	0	0	0	0
25	G	1	0	0	0	0
25	J	2	0	0	0	0
25	K	1	0	0	0	0
25	L	2	0	0	0	0
25	P	1	0	0	0	0
25	Q	2	0	0	0	0
25	R	1	0	0	0	0
25	T	1	0	0	0	0
25	V	1	0	0	0	0
25	W	4	0	0	0	0
25	X	6	0	0	0	0
26	A	30	0	0	2	0
27	D	8	0	0	0	0
28	N	1	0	0	0	0
29	X	1	0	0	0	0
30	A	204	0	0	12	0
30	D	1	0	0	0	0
30	G	1	0	0	1	0
30	I	1	0	0	0	0
30	J	4	0	0	0	0
30	L	4	0	0	0	0
30	O	1	0	0	0	0
30	P	1	0	0	0	0
30	R	1	0	0	0	0
30	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	W	2	0	0	0	0
30	X	6	0	0	0	0
All	All	56383	0	37865	1086	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 12.

All (1086) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1002:G:H1	1:A:1038:C:N4	1.51	1.08
1:A:1028:C:N3	1:A:1033:G:C6	2.23	1.06
1:A:1029:C:C4	1:A:1032:G:N1	2.32	0.97
23:W:50:U:H3	23:W:64:A:N6	1.63	0.97
1:A:947:G:H1	1:A:1234:C:H42	0.97	0.96
1:A:1132:C:H42	1:A:1142:G:H1	1.14	0.95
1:A:999:C:H42	1:A:1042:G:H1	1.10	0.95
23:W:27:G:H1	23:W:43:C:H42	1.12	0.93
1:A:38:G:H22	1:A:397:A:H5'	1.32	0.93
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.00	0.93
23:Y:19:G:N2	23:Y:56:C:N3	2.19	0.91
13:M:122:LYS:HD3	13:M:123:ALA:H	1.37	0.89
1:A:1002:G:N2	1:A:1038:C:N3	2.20	0.89
1:A:947:G:H1	1:A:1234:C:N4	1.70	0.88
23:W:50:U:H3	23:W:64:A:H61	0.89	0.88
1:A:1353:G:OP1	21:U:10:ARG:NH1	2.07	0.87
23:Y:29:G:H1	23:Y:41:C:H42	1.23	0.87
2:B:16:HIS:HB2	2:B:204:ASN:HB3	1.57	0.86
1:A:656:C:O2'	15:O:28:GLN:NE2	2.07	0.86
15:O:54:ARG:NH1	15:O:58:MET:SD	2.48	0.86
1:A:999:C:N4	1:A:1042:G:H1	1.73	0.86
2:B:18:GLY:HA2	2:B:42:ILE:HG13	1.55	0.86
3:C:41:GLY:O	3:C:45:LYS:NZ	2.09	0.85
5:E:143:ARG:NH1	8:H:77:GLU:OE1	2.09	0.85
5:E:100:VAL:O	5:E:107:ARG:NH2	2.10	0.83
1:A:1003:G:N2	1:A:1025:U:O4	2.11	0.83
1:A:1360:A:OP2	14:N:35:ARG:NH2	2.12	0.83
1:A:1029:C:N3	1:A:1032:G:N2	2.27	0.83
1:A:1502:A:H2	1:A:1505:G:H1	1.27	0.82
1:A:1028:C:C2	1:A:1033:G:C6	2.68	0.81
23:Y:26:A:N1	23:Y:44:G:C6	2.48	0.81
1:A:1002:G:H1	1:A:1038:C:H42	0.83	0.80
1:A:953:G:H5'	1:A:965:A:H61	1.45	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1003:G:O6	1:A:1035:A:N6	2.13	0.80
1:A:1029:C:N4	1:A:1032:G:N1	2.31	0.79
1:A:992:U:H3	1:A:1044:A:H62	1.26	0.79
1:A:522:C:H41	12:L:53:ARG:HH22	1.30	0.79
23:W:27:G:H1	23:W:43:C:N4	1.80	0.78
23:Y:5:G:H1	23:Y:68:C:H42	1.28	0.78
1:A:742:G:OP2	15:O:35:ARG:NH2	2.17	0.78
24:X:6:G:H1	24:X:67:C:H42	1.30	0.77
11:K:99:GLN:HG2	11:K:105:VAL:HG21	1.66	0.77
23:Y:26:A:N1	23:Y:44:G:O6	2.18	0.77
1:A:148:G:H2'	1:A:149:A:H8	1.49	0.77
23:W:4:C:N3	23:W:69:G:N2	2.33	0.77
1:A:975:A:H4'	1:A:976:G:H5''	1.67	0.77
1:A:427:U:OP1	4:D:13:ARG:NH2	2.18	0.76
23:Y:19:G:N1	23:Y:56:C:N4	2.34	0.76
4:D:98:GLU:OE1	4:D:103:ASN:ND2	2.16	0.76
2:B:88:ALA:HB1	2:B:222:ILE:HD11	1.67	0.76
4:D:165:MET:SD	4:D:168:ARG:NH1	2.58	0.76
9:I:117:HIS:HB2	9:I:121:ARG:HG2	1.68	0.76
1:A:1329:A:H5''	13:M:26:GLY:H	1.51	0.76
1:A:158:G:N2	1:A:163:C:O2	2.19	0.75
13:M:58:GLU:O	13:M:62:ASN:ND2	2.18	0.75
13:M:3:ARG:NH2	13:M:9:ILE:O	2.18	0.75
1:A:1029:C:C2	1:A:1032:G:N2	2.55	0.75
1:A:1256:A:N6	1:A:1278:U:O2	2.20	0.75
8:H:51:VAL:HG21	8:H:60:ARG:HB2	1.67	0.75
9:I:7:THR:O	9:I:83:ARG:NH1	2.20	0.75
23:Y:18:G:N2	23:Y:55:PSU:N3	2.34	0.75
1:A:1132:C:N4	1:A:1142:G:H1	1.86	0.74
1:A:504:C:OP1	30:A:4006:HOH:O	2.05	0.74
1:A:1301:U:O2'	1:A:1302:U:H5'	1.88	0.74
1:A:922:G:H4'	5:E:20:GLN:HA	1.69	0.74
22:V:23:A:H4'	22:V:24:A:H5'	1.70	0.74
13:M:13:LYS:HA	13:M:44:ARG:HH11	1.53	0.74
1:A:860:A:OP2	30:A:4160:HOH:O	2.04	0.73
13:M:107:ALA:HB3	13:M:111:LYS:HD2	1.68	0.73
10:J:11:PHE:HE1	10:J:67:THR:HG22	1.52	0.73
23:Y:51:U:H3	23:Y:63:G:H1	1.36	0.73
1:A:1279:A:O2'	1:A:1281:U:OP2	2.06	0.73
1:A:1029:C:N4	1:A:1032:G:C6	2.57	0.73
1:A:582:U:OP1	15:O:68:ARG:NH2	2.20	0.73
1:A:21:G:OP1	30:A:4063:HOH:O	2.06	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:29:G:H1	23:Y:41:C:N4	1.87	0.73
1:A:770:C:OP1	30:A:4118:HOH:O	2.06	0.72
16:P:52:ASP:O	16:P:54:GLU:N	2.22	0.72
20:T:57:ARG:HH22	20:T:100:ILE:HD12	1.50	0.72
1:A:1244:C:H42	1:A:1293:G:H1	1.37	0.72
12:L:57:LYS:NZ	12:L:65:GLU:OE2	2.21	0.72
9:I:53:VAL:O	9:I:55:ALA:N	2.22	0.71
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.24	0.71
2:B:201:ILE:HG21	2:B:214:ILE:HG21	1.73	0.71
15:O:4:THR:OG1	15:O:7:GLU:OE1	2.08	0.71
1:A:64:G:H4'	1:A:65:U:H3'	1.72	0.71
13:M:4:ILE:HG23	13:M:5:ALA:H	1.55	0.71
1:A:664:G:H22	1:A:741:G:H1	1.38	0.70
1:A:1314:C:OP2	19:S:4:SER:OG	2.07	0.70
7:G:136:LYS:NZ	7:G:139:GLU:OE2	2.24	0.70
1:A:1029:C:C4	1:A:1032:G:C2	2.80	0.70
1:A:1028:C:C4	1:A:1033:G:O6	2.44	0.70
1:A:1163:C:H42	1:A:1173:G:H1	1.40	0.70
7:G:80:VAL:HB	7:G:85:TYR:HE2	1.57	0.70
1:A:1129:C:H42	1:A:1143:G:H1	1.40	0.70
2:B:47:THR:HA	2:B:202:PRO:HG2	1.74	0.70
10:J:52:GLY:O	14:N:41:ARG:NH2	2.24	0.70
2:B:120:ALA:O	2:B:122:PHE:N	2.21	0.70
13:M:39:ILE:HD12	13:M:52:GLU:HG2	1.73	0.70
1:A:1151:A:HO2'	1:A:1152:A:H8	1.37	0.70
8:H:69:ARG:NH2	8:H:75:ARG:O	2.23	0.70
1:A:1148:U:O2'	9:I:66:ARG:NH2	2.25	0.70
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.74	0.69
1:A:677:U:H3	1:A:713:G:H22	1.39	0.69
1:A:1104:G:O3'	2:B:111:ARG:NH2	2.25	0.69
1:A:1024:G:H2'	1:A:1025:U:H5''	1.73	0.69
10:J:17:ASP:OD1	10:J:70:ARG:NH1	2.26	0.69
1:A:1027:C:C2	1:A:1034:G:N1	2.57	0.69
1:A:1228:C:OP2	13:M:108:ARG:NH2	2.20	0.69
1:A:1159:U:O4'	1:A:1182:G:N2	2.26	0.69
9:I:128:ARG:NH2	24:X:33:U:OP2	2.26	0.69
23:W:4:C:N4	23:W:69:G:N1	2.40	0.69
18:R:32:ARG:HA	18:R:69:THR:HG21	1.75	0.68
1:A:1010:G:N2	1:A:1020:U:H1'	2.09	0.68
1:A:539:A:OP2	12:L:115:LYS:NZ	2.26	0.68
23:Y:7:A:H61	23:Y:66:U:H3	1.42	0.68
1:A:1010:G:H2'	1:A:1011:G:H8	1.59	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1152:A:H5'	10:J:13:HIS:HB2	1.75	0.68
10:J:44:VAL:HG13	10:J:66:ARG:HG2	1.75	0.68
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.27	0.67
1:A:1312:G:H5'	19:S:5:LEU:HD21	1.77	0.67
1:A:36:C:OP1	12:L:123:LYS:NZ	2.28	0.67
1:A:999:C:N3	1:A:1042:G:N2	2.37	0.67
13:M:88:ARG:HG3	13:M:98:VAL:HG11	1.76	0.67
11:K:48:ILE:O	11:K:50:TYR:N	2.28	0.67
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.76	0.67
1:A:1028:C:C2	1:A:1033:G:N1	2.62	0.67
1:A:148:G:H2'	1:A:149:A:C8	2.30	0.67
9:I:9:ARG:HG2	9:I:14:VAL:HG12	1.75	0.67
1:A:1129:C:H2'	1:A:1139:G:N7	2.10	0.67
5:E:50:GLU:HB2	5:E:53:LEU:HD13	1.76	0.67
9:I:23:ASN:ND2	9:I:25:LYS:HG2	2.10	0.66
18:R:56:THR:HB	18:R:58:LEU:HD23	1.77	0.66
1:A:1129:C:N4	1:A:1143:G:H1	1.93	0.66
3:C:100:ALA:O	3:C:102:ASN:ND2	2.28	0.66
9:I:102:LEU:HD13	9:I:103:THR:H	1.59	0.66
9:I:3:GLN:OE1	9:I:20:ARG:NH2	2.25	0.66
1:A:1064:G:N2	1:A:1190:G:O2'	2.29	0.66
2:B:125:PRO:O	2:B:127:ILE:N	2.28	0.66
1:A:38:G:N2	1:A:397:A:H5''	2.09	0.66
1:A:79:G:H1	1:A:90:U:H3	1.44	0.66
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.77	0.66
20:T:10:LEU:HB3	20:T:12:ALA:H	1.60	0.65
1:A:1166:G:N2	1:A:1170:A:OP2	2.29	0.65
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.29	0.65
14:N:4:LYS:HA	14:N:7:ILE:HG22	1.77	0.65
16:P:51:VAL:HG12	16:P:53:VAL:H	1.61	0.65
1:A:390:C:O3'	16:P:28:ARG:NH2	2.29	0.65
1:A:947:G:N2	1:A:1234:C:N3	2.42	0.65
1:A:426:G:OP1	4:D:38:TYR:OH	2.12	0.65
24:X:47:U:N3	24:X:50:U:OP1	2.30	0.65
23:W:50:U:H6	23:W:50:U:H5'	1.62	0.65
1:A:377:G:OP1	16:P:3:LYS:HD2	1.97	0.65
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.77	0.65
4:D:175:SER:HB3	4:D:186:LEU:HD11	1.79	0.65
13:M:78:ILE:HA	13:M:81:LEU:HD12	1.79	0.64
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.78	0.64
23:Y:15:G:H22	23:Y:48:C:H42	1.44	0.64
1:A:411:A:OP2	4:D:25:ARG:NH2	2.29	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1108:G:O6	30:A:4094:HOH:O	2.11	0.64
1:A:954:G:H21	1:A:1227:A:H62	1.45	0.64
2:B:15:VAL:HG21	2:B:213:LEU:HD12	1.79	0.64
3:C:164:ARG:NH1	3:C:166:GLU:OE1	2.31	0.64
1:A:8:A:H5'	5:E:101:ILE:HG22	1.79	0.64
10:J:38:ILE:HD11	10:J:71:LEU:HD23	1.79	0.64
1:A:1027:C:N3	1:A:1034:G:O6	2.30	0.64
1:A:1119:C:H42	1:A:1154:G:H1	1.44	0.64
2:B:78:GLN:NE2	2:B:95:GLN:OE1	2.30	0.64
1:A:1028:C:N3	1:A:1033:G:O6	2.30	0.64
1:A:1251:A:H2'	1:A:1252:A:C8	2.33	0.64
6:F:70:ASP:N	6:F:70:ASP:OD1	2.28	0.64
1:A:559:A:OP1	5:E:126:ARG:NH2	2.27	0.64
2:B:178:ARG:HH22	8:H:68:ARG:NH1	1.96	0.63
1:A:572:A:OP1	30:A:4047:HOH:O	2.15	0.63
24:X:31:G:H3'	24:X:32:5MC:HM51	1.81	0.63
1:A:1278:U:H5'	1:A:1279:A:O4'	1.98	0.63
1:A:1026:G:H5'	1:A:1027:C:O5'	1.98	0.63
1:A:254:G:OP1	17:Q:66:SER:OG	2.09	0.63
1:A:1027:C:O2	1:A:1034:G:N1	2.30	0.63
1:A:1039:C:H2'	1:A:1040:U:O4'	1.99	0.63
1:A:811:C:O2'	1:A:901:A:N1	2.30	0.63
20:T:9:ASN:O	20:T:10:LEU:HB2	1.99	0.62
1:A:1499:A:H1'	1:A:1520:G:H5'	1.81	0.62
2:B:155:LEU:HD21	2:B:159:PRO:HG3	1.80	0.62
23:Y:44:G:H2'	23:Y:45:U:H5'	1.81	0.62
9:I:20:ARG:O	9:I:60:ASP:N	2.29	0.62
23:Y:18:G:N2	23:Y:55:PSU:C4	2.66	0.62
1:A:1010:G:H2'	1:A:1011:G:C8	2.35	0.62
1:A:881:G:P	12:L:12:ARG:HH22	2.22	0.62
23:W:51:U:H2'	23:W:52:G:C8	2.35	0.62
1:A:1221:G:OP1	1:A:1320:C:N4	2.33	0.62
2:B:187:LEU:HA	2:B:201:ILE:HB	1.81	0.62
1:A:406:G:H5'	4:D:5:ILE:HD11	1.82	0.62
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.82	0.62
1:A:771:G:N7	30:A:4039:HOH:O	2.30	0.62
1:A:1502:A:H2	1:A:1505:G:N1	1.94	0.62
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.81	0.62
23:Y:11:C:N3	23:Y:24:G:O6	2.33	0.62
5:E:52:PRO:HG2	5:E:53:LEU:HD12	1.82	0.61
1:A:448:A:P	1:A:485:G:H22	2.23	0.61
4:D:166:LYS:NZ	4:D:179:GLU:OE2	2.32	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:14:ARG:HG2	8:H:18:ARG:HH22	1.66	0.61
1:A:1027:C:C4	1:A:1034:G:O6	2.53	0.61
1:A:1240:U:N3	7:G:30:ILE:O	2.29	0.61
1:A:564:C:O2'	8:H:91:ARG:NH2	2.31	0.61
1:A:920:U:H2'	1:A:921:U:C6	2.36	0.61
23:Y:14:A:O2'	23:Y:15:G:OP1	2.17	0.61
1:A:1005:A:H5''	1:A:1006:C:C5	2.35	0.61
1:A:1055:A:N7	1:A:1200:C:N4	2.49	0.61
1:A:986:A:N3	19:S:52:TYR:OH	2.31	0.61
1:A:1028:C:O2	1:A:1033:G:N1	2.34	0.61
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.82	0.61
1:A:17:U:H2'	1:A:18:C:C6	2.36	0.61
1:A:854:G:O6	30:A:4130:HOH:O	2.16	0.61
4:D:88:VAL:HG13	5:E:97:GLY:HA2	1.83	0.61
23:Y:5:G:H1	23:Y:68:C:N4	1.97	0.61
1:A:1010:G:H22	1:A:1020:U:H1'	1.65	0.60
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.81	0.60
24:X:6:G:H1	24:X:67:C:N4	1.97	0.60
5:E:140:ARG:O	5:E:143:ARG:NH2	2.35	0.60
1:A:1120:G:C5	1:A:1154:G:N2	2.70	0.60
20:T:10:LEU:HD23	20:T:12:ALA:HB2	1.83	0.60
8:H:119:LEU:HB3	8:H:123:GLU:HB3	1.82	0.60
1:A:1126:U:H3	10:J:40:LEU:HD11	1.66	0.60
11:K:22:HIS:HB3	11:K:29:ILE:HB	1.84	0.60
23:W:13:C:O2'	23:W:14:A:O5'	2.16	0.60
23:Y:50:U:O2	23:Y:64:A:N1	2.34	0.60
1:A:6:G:H4'	1:A:298:A:H4'	1.84	0.60
1:A:1183:A:O2'	1:A:1184:G:OP1	2.16	0.59
1:A:1286:A:C8	1:A:1287:A:H4'	2.37	0.59
1:A:1086:U:H3	1:A:1099:G:H22	1.47	0.59
1:A:1103:C:OP1	2:B:96:ARG:NH2	2.34	0.59
1:A:1029:C:N3	1:A:1032:G:C2	2.70	0.59
1:A:67:C:H2'	1:A:68:G:C8	2.37	0.59
1:A:1128:C:H1'	1:A:1147:C:H42	1.67	0.59
3:C:19:GLU:HA	3:C:54:ARG:HH22	1.68	0.59
23:W:43:C:H2'	23:W:44:G:C8	2.36	0.59
4:D:147:ALA:HB2	4:D:182:LYS:HG3	1.85	0.59
13:M:37:THR:O	13:M:55:ARG:NH1	2.36	0.59
23:W:25:C:H2'	23:W:26:A:H5''	1.84	0.59
1:A:1286:A:H2'	1:A:1287:A:H4'	1.85	0.58
1:A:344:A:H5''	1:A:345:C:H5	1.68	0.58
1:A:942:G:H21	9:I:124:GLN:NE2	2.01	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1503:A:O2'	22:V:13:A:N1	2.35	0.58
23:Y:51:U:H2'	23:Y:52:G:O4'	2.03	0.58
1:A:1147:C:H1'	9:I:16:ARG:HH21	1.68	0.58
1:A:662:G:H2'	1:A:663:A:C8	2.38	0.58
1:A:1119:C:OP2	9:I:9:ARG:NH1	2.37	0.58
1:A:673:G:H2'	1:A:674:G:C8	2.38	0.58
15:O:4:THR:N	15:O:7:GLU:OE2	2.35	0.58
23:W:44:G:H8	23:W:44:G:O5'	1.87	0.58
23:W:61:C:O2'	23:W:62:C:O5'	2.12	0.58
5:E:71:LEU:HD11	5:E:115:VAL:HG22	1.85	0.58
23:Y:36:A:H2'	23:Y:37:MIA:O4'	2.03	0.58
1:A:976:G:H5'	1:A:1358:U:O2'	2.04	0.58
23:W:63:G:H2'	23:W:64:A:O4'	2.04	0.58
1:A:1133:G:H2'	1:A:1134:G:O4'	2.04	0.58
1:A:1348:U:H4'	9:I:120:ARG:HD2	1.86	0.58
1:A:1244:C:N4	1:A:1293:G:H1	2.00	0.57
2:B:185:ILE:HG22	2:B:199:TYR:HD2	1.69	0.57
7:G:27:ILE:HD12	7:G:40:ALA:HA	1.85	0.57
5:E:43:LEU:HD21	5:E:132:ALA:HB1	1.86	0.57
15:O:5:LYS:N	15:O:5:LYS:HD3	2.19	0.57
23:W:4:C:N4	23:W:69:G:H1	2.02	0.57
23:W:2:C:N3	23:W:71:G:O6	2.37	0.57
10:J:5:ARG:N	10:J:99:LYS:O	2.37	0.57
1:A:978:A:O2'	1:A:1322:C:N3	2.31	0.57
23:Y:50:U:C2	23:Y:64:A:N1	2.73	0.57
24:X:5:G:H1	24:X:68:C:H42	1.52	0.57
4:D:162:LEU:HD13	4:D:181:MET:HG2	1.85	0.57
1:A:1054:C:C4	23:W:34:G:H1'	2.40	0.57
2:B:131:PRO:O	2:B:135:GLN:HB2	2.05	0.56
19:S:30:LEU:HD11	19:S:50:ALA:HB2	1.87	0.56
1:A:1239:A:H4'	1:A:1240:U:H5''	1.88	0.56
1:A:1348:U:H2'	1:A:1349:A:H8	1.70	0.56
1:A:828:A:OP1	8:H:21:LYS:NZ	2.38	0.56
17:Q:95:TYR:HA	17:Q:98:LEU:HD12	1.85	0.56
1:A:1004:A:N6	1:A:1037:C:C2	2.74	0.56
9:I:110:GLU:OE2	9:I:113:LYS:NZ	2.38	0.56
3:C:71:ALA:HA	3:C:106:VAL:HB	1.88	0.56
9:I:9:ARG:O	9:I:104:ARG:HG3	2.06	0.56
1:A:1255:G:OP1	10:J:45:ARG:NH2	2.35	0.56
12:L:117:ARG:HB3	12:L:122:THR:O	2.04	0.56
1:A:1064:G:O6	1:A:1191:A:N6	2.39	0.56
1:A:1305:G:N2	1:A:1331:G:H1'	2.20	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:157:LEU:O	4:D:161:ASN:ND2	2.38	0.56
7:G:113:GLU:CG	7:G:119:ARG:HG2	2.36	0.56
19:S:28:LYS:HB3	19:S:29:ARG:HA	1.88	0.56
1:A:1151:A:O2'	1:A:1152:A:H8	1.88	0.56
2:B:73:THR:HA	2:B:94:ASN:O	2.06	0.56
3:C:43:LEU:HD21	3:C:91:LEU:HD13	1.88	0.56
8:H:14:ARG:HG2	8:H:18:ARG:NH2	2.20	0.56
11:K:85:ARG:HD3	11:K:113:PRO:HD3	1.88	0.56
3:C:152:ILE:HG23	3:C:199:LYS:HB2	1.87	0.56
13:M:91:ARG:HB2	13:M:98:VAL:HG13	1.87	0.56
23:Y:19:G:C2	23:Y:56:C:N3	2.74	0.56
23:Y:19:G:C6	23:Y:56:C:N4	2.73	0.56
2:B:233:SER:HB2	2:B:234:PRO:HD2	1.86	0.56
19:S:27:GLU:HG2	19:S:47:HIS:CE1	2.40	0.56
1:A:1028:C:O2	1:A:1033:G:C2	2.60	0.55
8:H:41:ARG:NH2	8:H:123:GLU:OE2	2.38	0.55
1:A:1221:G:O3'	19:S:77:THR:OG1	2.24	0.55
1:A:1239:A:H62	1:A:1299:A:H62	1.52	0.55
1:A:256:U:OP1	17:Q:17:LYS:NZ	2.34	0.55
1:A:646:U:H2'	1:A:647:C:C6	2.42	0.55
3:C:26:LYS:HG3	10:J:45:ARG:HH12	1.72	0.55
1:A:450:G:OP1	16:P:43:LYS:NZ	2.38	0.55
1:A:532:A:H2	1:A:1206:G:H21	1.54	0.55
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.71	0.55
1:A:1318:A:OP1	19:S:3:ARG:NH2	2.38	0.55
3:C:52:LEU:HD11	3:C:55:VAL:HG23	1.88	0.55
23:Y:9:A:H5'	23:Y:46:7MG:N3	2.22	0.55
2:B:144:ARG:NH2	2:B:148:TYR:OH	2.39	0.55
1:A:1075:C:OP1	2:B:179:LYS:NZ	2.31	0.55
1:A:1299:A:H2'	1:A:1299:A:N3	2.22	0.55
1:A:538:G:H5''	12:L:114:LYS:HB2	1.88	0.55
15:O:5:LYS:O	15:O:9:GLN:HG2	2.07	0.55
1:A:942:G:H21	9:I:124:GLN:HE22	1.54	0.55
23:W:27:G:N2	23:W:43:C:N3	2.48	0.55
1:A:1028:C:C4	1:A:1033:G:C6	2.94	0.55
1:A:1060:C:N4	3:C:2:GLY:HA2	2.22	0.55
3:C:79:ARG:O	3:C:82:GLU:HB2	2.06	0.55
1:A:953:G:H5'	1:A:965:A:N6	2.19	0.55
1:A:973:G:H3'	1:A:974:A:H5''	1.88	0.55
12:L:117:ARG:NH2	12:L:124:LYS:HG2	2.22	0.55
3:C:179:ARG:NH1	3:C:206:GLU:OE1	2.40	0.54
19:S:63:THR:OG1	19:S:65:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:U:H2'	1:A:46:G:C8	2.42	0.54
1:A:1288:A:N1	1:A:1371:G:H1'	2.21	0.54
1:A:54:C:N4	1:A:353:A:OP2	2.38	0.54
2:B:178:ARG:HH22	8:H:68:ARG:HH12	1.56	0.54
20:T:53:LEU:HA	20:T:56:MET:HG2	1.90	0.54
1:A:157:G:H1	1:A:164:U:H3	1.54	0.54
9:I:81:ILE:O	9:I:85:LEU:HG	2.08	0.54
3:C:138:VAL:HG23	3:C:151:VAL:HG23	1.90	0.54
1:A:1028:C:N3	1:A:1033:G:C5	2.74	0.54
4:D:58:LEU:HD22	4:D:62:GLN:HG2	1.90	0.54
4:D:6:GLY:H	4:D:115:ARG:HH12	1.56	0.54
13:M:90:LEU:HD23	13:M:93:ARG:HE	1.73	0.54
1:A:396:G:O2'	1:A:398:C:OP1	2.16	0.54
1:A:93:G:O2'	1:A:96:U:H5'	2.07	0.54
24:X:50:U:H3	24:X:64:G:H1	1.53	0.54
23:Y:50:U:N3	23:Y:64:A:N6	2.55	0.54
1:A:684:A:N6	30:A:4138:HOH:O	2.40	0.54
16:P:58:TYR:O	16:P:61:SER:OG	2.19	0.54
1:A:1456:G:O3'	20:T:39:LYS:NZ	2.41	0.54
1:A:375:U:OP1	16:P:69:THR:HG21	2.08	0.53
9:I:9:ARG:H	9:I:79:LEU:HD23	1.73	0.53
23:W:21:A:N6	23:W:46:7MG:C4	2.77	0.53
1:A:328:C:H4'	1:A:329:A:H5'	1.91	0.53
1:A:93:G:C2'	1:A:96:U:H5'	2.38	0.53
6:F:23:LYS:HG2	6:F:61:LEU:HD21	1.90	0.53
10:J:12:ASP:OD2	10:J:15:THR:HG23	2.08	0.53
20:T:18:GLN:O	20:T:22:ARG:HG3	2.08	0.53
1:A:1149:C:H2'	1:A:1150:U:C6	2.43	0.53
1:A:1148:U:H2'	1:A:1149:C:O4'	2.08	0.53
1:A:1249:C:O4'	9:I:70:LYS:NZ	2.42	0.53
2:B:15:VAL:HG13	2:B:209:ARG:HB3	1.90	0.53
1:A:1118:C:OP1	9:I:104:ARG:NH1	2.42	0.53
24:X:66:C:H2'	24:X:67:C:O4'	2.08	0.53
23:Y:52:G:O6	23:Y:62:C:N3	2.41	0.53
23:Y:58:A:H1'	23:Y:60:U:H3	1.72	0.53
2:B:77:ALA:HA	2:B:80:ILE:HG22	1.90	0.53
9:I:8:GLY:O	9:I:14:VAL:HA	2.08	0.53
1:A:1152:A:OP1	10:J:70:ARG:NH2	2.42	0.53
23:W:28:G:H2'	23:W:29:G:O4'	2.08	0.53
1:A:1192:C:OP1	3:C:4:LYS:NZ	2.41	0.53
19:S:52:TYR:HB2	19:S:57:HIS:CE1	2.43	0.53
24:X:15:G:H2'	24:X:59:A:N1	2.24	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:176:LEU:HD12	4:D:182:LYS:O	2.08	0.53
12:L:83:VAL:HG23	12:L:107:ALA:HB2	1.90	0.53
1:A:56:U:H2'	1:A:57:G:C8	2.43	0.53
1:A:757:U:H2'	1:A:758:G:O4'	2.09	0.53
10:J:42:THR:HG23	10:J:68:HIS:HA	1.91	0.53
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.91	0.53
15:O:6:GLU:OE2	15:O:6:GLU:N	2.39	0.53
23:Y:18:G:N1	23:Y:55:PSU:C4	2.76	0.53
1:A:1121:U:C4	1:A:1122:U:C4	2.97	0.53
6:F:76:ALA:O	6:F:80:ARG:HG3	2.08	0.53
12:L:124:LYS:HD3	12:L:125:PRO:HD2	1.91	0.53
23:W:18:G:O2'	23:W:57:G:N2	2.33	0.53
23:W:50:U:H2'	23:W:51:U:C6	2.44	0.53
1:A:1002:G:C4	1:A:1003:G:C8	2.97	0.53
1:A:1435:G:H2'	1:A:1436:U:C6	2.44	0.53
1:A:838:G:H1	1:A:848:C:N4	2.07	0.53
8:H:46:LYS:HA	8:H:64:LYS:HE3	1.90	0.53
15:O:28:GLN:NE2	15:O:66:LEU:HD21	2.24	0.53
23:W:44:G:H2'	23:W:45:U:H5'	1.90	0.53
1:A:1060:C:H5''	10:J:51:ARG:HB3	1.91	0.53
1:A:1179:A:H4'	9:I:103:THR:HA	1.91	0.53
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.91	0.53
10:J:32:ALA:HB1	10:J:33:GLN:HG2	1.91	0.53
1:A:141:A:H1'	1:A:182:U:O2	2.09	0.52
2:B:21:ARG:HA	2:B:39:ILE:HD13	1.91	0.52
15:O:28:GLN:HE21	15:O:66:LEU:HD21	1.73	0.52
1:A:1151:A:H5''	10:J:41:PRO:HA	1.92	0.52
1:A:200:G:H2'	1:A:201:C:O4'	2.09	0.52
1:A:976:G:OP1	14:N:32:SER:N	2.38	0.52
1:A:1246:C:H2'	1:A:1247:U:H6	1.74	0.52
1:A:825:G:H21	8:H:11:THR:HG21	1.73	0.52
18:R:22:VAL:HB	18:R:56:THR:HA	1.92	0.52
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.91	0.52
1:A:353:A:H5'	1:A:353:A:H8	1.74	0.52
4:D:72:GLU:OE1	4:D:207:TYR:OH	2.25	0.52
1:A:986:A:H1'	19:S:55:LYS:HA	1.90	0.52
13:M:40:ASN:ND2	13:M:41:PRO:HD2	2.24	0.52
20:T:43:LEU:HD13	20:T:51:GLU:HB3	1.92	0.52
1:A:441:A:H5'	1:A:442:C:OP2	2.10	0.52
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.92	0.52
11:K:45:GLY:O	11:K:50:TYR:HB2	2.10	0.52
1:A:1048:G:OP1	14:N:3:ARG:NH2	2.40	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1087:G:N2	1:A:1099:G:H1'	2.25	0.52
1:A:1360:A:OP1	1:A:1360:A:H8	1.92	0.52
1:A:1352:C:H2'	1:A:1353:G:C8	2.45	0.52
1:A:473:G:H2'	1:A:474:G:H8	1.75	0.52
1:A:828:A:H5''	1:A:859:A:C2	2.44	0.52
3:C:113:ALA:N	3:C:183:ASP:OD2	2.39	0.52
1:A:1202:G:O4'	14:N:29:ARG:NH1	2.42	0.52
23:Y:15:G:N2	23:Y:48:C:H42	2.07	0.52
1:A:1042:G:H2'	1:A:1043:C:O4'	2.10	0.52
1:A:1152:A:C5'	10:J:13:HIS:HB2	2.39	0.52
2:B:167:PRO:HG2	2:B:192:SER:HB2	1.91	0.52
2:B:16:HIS:HB2	2:B:204:ASN:CB	2.35	0.52
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.91	0.52
1:A:1134:G:H2'	1:A:1135:U:H5'	1.92	0.52
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.92	0.52
4:D:18:LYS:NZ	4:D:31:CYS:SG	2.83	0.52
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.92	0.52
1:A:356:A:N3	1:A:368:U:O2'	2.37	0.51
3:C:6:HIS:HD2	3:C:8:ILE:H	1.58	0.51
4:D:157:LEU:HD22	4:D:161:ASN:HD21	1.74	0.51
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.91	0.51
1:A:222:U:H2'	1:A:223:U:C6	2.45	0.51
1:A:344:A:H5''	1:A:345:C:C5	2.44	0.51
15:O:26:GLU:OE2	15:O:77:ARG:NE	2.37	0.51
23:W:51:U:H2'	23:W:52:G:H8	1.75	0.51
23:Y:66:U:H2'	23:Y:67:C:O4'	2.10	0.51
1:A:1095:U:H5''	1:A:1109:C:O2	2.10	0.51
1:A:922:G:N3	1:A:1398:A:H2	2.08	0.51
2:B:178:ARG:NH1	2:B:196:LEU:O	2.43	0.51
2:B:76:GLN:H	2:B:76:GLN:CD	2.14	0.51
20:T:50:GLU:HB2	20:T:99:LEU:HD23	1.92	0.51
1:A:1095:U:P	1:A:1108:G:H1	2.34	0.51
1:A:1218:C:H2'	1:A:1219:U:C6	2.46	0.51
8:H:82:HIS:NE2	8:H:84:ARG:HG2	2.25	0.51
1:A:1013:G:N2	1:A:1016:A:OP2	2.43	0.51
11:K:20:TYR:CZ	11:K:83:ILE:HD12	2.46	0.51
1:A:1041:A:H2'	1:A:1042:G:C8	2.45	0.51
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.92	0.51
7:G:113:GLU:HG3	7:G:119:ARG:HG2	1.93	0.51
1:A:192:U:H2'	1:A:193:C:C6	2.46	0.51
2:B:16:HIS:CB	2:B:204:ASN:HB3	2.37	0.51
3:C:77:ILE:O	3:C:84:ILE:N	2.41	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.92	0.51
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.46	0.50
23:Y:13:C:H2'	23:Y:14:A:H5''	1.93	0.50
1:A:1006:C:H2'	1:A:1007:C:C6	2.47	0.50
1:A:170:U:O2'	1:A:171:A:H5'	2.11	0.50
1:A:392:G:H2'	1:A:393:A:H8	1.75	0.50
2:B:16:HIS:HB3	2:B:210:SER:CB	2.40	0.50
3:C:37:GLN:NE2	14:N:52:GLN:OE1	2.44	0.50
9:I:16:ARG:HB2	9:I:64:THR:HB	1.92	0.50
23:Y:15:G:H22	23:Y:48:C:N4	2.09	0.50
1:A:1163:C:N4	1:A:1173:G:H1	2.07	0.50
1:A:1376:U:H2'	1:A:1377:A:C8	2.46	0.50
1:A:297:G:N2	1:A:300:A:OP2	2.43	0.50
10:J:37:PRO:HA	10:J:72:VAL:HG12	1.93	0.50
1:A:1412:C:H2'	1:A:1413:A:C8	2.46	0.50
2:B:9:GLU:O	2:B:11:LEU:N	2.45	0.50
4:D:25:ARG:NH1	4:D:30:LYS:O	2.44	0.50
7:G:132:GLY:O	7:G:136:LYS:HG2	2.12	0.50
1:A:1226:C:H4'	19:S:80:TYR:CZ	2.47	0.50
1:A:537:G:H2'	1:A:538:G:C8	2.47	0.50
23:Y:62:C:H2'	23:Y:63:G:C8	2.47	0.50
1:A:1039:C:N4	1:A:1040:U:C4	2.80	0.50
1:A:250:A:H4'	1:A:251:G:O5'	2.11	0.50
4:D:15:GLU:OE2	4:D:66:ARG:NH1	2.44	0.50
1:A:1227:A:OP2	13:M:111:LYS:NZ	2.33	0.50
1:A:1034:G:H3'	1:A:1035:A:C8	2.47	0.50
19:S:77:THR:HG22	19:S:78:ARG:HG2	1.94	0.50
1:A:1051:C:H2'	1:A:1052:U:C6	2.47	0.49
1:A:1053:G:N7	1:A:1200:C:H5''	2.26	0.49
3:C:43:LEU:HD11	3:C:91:LEU:HD11	1.94	0.49
3:C:131:ARG:NH1	5:E:50:GLU:HG3	2.25	0.49
1:A:918:A:H2'	1:A:919:A:O4'	2.13	0.49
1:A:1103:C:P	2:B:96:ARG:HH22	2.34	0.49
3:C:115:LEU:O	3:C:118:GLN:HG2	2.12	0.49
1:A:1285:A:H4'	1:A:1286:A:O5'	2.12	0.49
2:B:91:PRO:HA	2:B:151:GLY:O	2.12	0.49
3:C:122:GLU:HA	3:C:125:GLU:OE2	2.11	0.49
14:N:26:ARG:NH2	14:N:47:LEU:HD21	2.27	0.49
1:A:1136:U:OP2	1:A:1137:C:N4	2.46	0.49
1:A:1176:A:H2'	1:A:1177:G:O4'	2.12	0.49
1:A:447:G:O6	1:A:485:G:O2'	2.23	0.49
1:A:152:A:N6	1:A:169:C:N3	2.58	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:48:MET:HA	2:B:51:LEU:HD12	1.94	0.49
8:H:119:LEU:HD13	8:H:127:LEU:HD23	1.94	0.49
1:A:1009:G:N2	1:A:1010:G:H1'	2.27	0.49
1:A:1347:G:N2	1:A:1373:G:H2'	2.27	0.49
8:H:73:ASP:OD1	8:H:75:ARG:HD3	2.11	0.49
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.95	0.49
23:Y:23:A:H2'	23:Y:24:G:H5''	1.94	0.49
23:Y:58:A:N3	23:Y:60:U:N3	2.60	0.49
1:A:1024:G:H2'	1:A:1024:G:N3	2.27	0.49
1:A:646:U:H2'	1:A:647:C:H6	1.76	0.49
6:F:69:GLU:O	6:F:72:VAL:HG12	2.13	0.49
9:I:28:VAL:HG22	9:I:63:ILE:HB	1.93	0.49
9:I:89:ASN:O	9:I:92:TYR:HB2	2.13	0.49
23:Y:2:C:N3	23:Y:71:G:O6	2.46	0.49
1:A:1168:A:C6	1:A:1169:A:C6	3.00	0.49
1:A:1262:C:H2'	1:A:1263:C:H6	1.78	0.49
1:A:1359:C:H1'	1:A:1362:C:H41	1.78	0.49
2:B:162:ILE:HD11	2:B:184:VAL:HG22	1.94	0.49
12:L:60:LEU:HD21	12:L:66:VAL:HG22	1.93	0.49
1:A:49:U:O4	1:A:365:U:H5	1.96	0.49
19:S:30:LEU:HA	19:S:48:THR:O	2.13	0.49
19:S:51:VAL:O	19:S:58:VAL:N	2.35	0.49
1:A:1360:A:H2'	1:A:1361:G:O4'	2.13	0.48
1:A:750:G:H1'	15:O:22:THR:OG1	2.12	0.48
2:B:120:ALA:C	2:B:122:PHE:H	2.14	0.48
2:B:71:VAL:HB	2:B:164:VAL:HG13	1.94	0.48
1:A:1012:U:H2'	1:A:1013:G:C8	2.48	0.48
21:U:12:LYS:HZ1	21:U:19:GLY:HA3	1.78	0.48
23:Y:44:G:C2'	23:Y:45:U:H5'	2.44	0.48
1:A:1002:G:N3	1:A:1003:G:C8	2.81	0.48
1:A:1352:C:OP1	21:U:3:LYS:NZ	2.36	0.48
1:A:692:U:O2'	1:A:694:A:N7	2.25	0.48
2:B:144:ARG:O	2:B:147:LYS:HB3	2.13	0.48
2:B:230:VAL:HG22	2:B:231:GLU:H	1.77	0.48
6:F:68:PRO:HG2	6:F:71:ARG:NH1	2.29	0.48
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.94	0.48
1:A:1273:G:H3'	1:A:1274:G:H8	1.78	0.48
2:B:211:ILE:O	2:B:215:LEU:HB2	2.13	0.48
2:B:80:ILE:HD11	2:B:212:GLN:HA	1.96	0.48
2:B:213:LEU:HD22	2:B:214:ILE:HD13	1.94	0.48
13:M:106:ASN:C	13:M:108:ARG:H	2.16	0.48
1:A:1258:G:O2'	1:A:1259:C:H5'	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:397:A:N3	1:A:397:A:H3'	2.28	0.48
1:A:22:G:H4'	1:A:885:G:C8	2.48	0.48
1:A:946:A:H2'	1:A:947:G:C8	2.49	0.48
3:C:85:ARG:O	3:C:89:GLU:N	2.44	0.48
8:H:69:ARG:HD3	8:H:75:ARG:O	2.14	0.48
23:Y:7:A:N6	23:Y:66:U:H3	2.08	0.48
1:A:1005:A:C8	1:A:1024:G:N2	2.82	0.48
1:A:1221:G:C2'	1:A:1222:G:H5'	2.44	0.48
1:A:1308:U:OP1	13:M:98:VAL:HG23	2.13	0.48
3:C:23:TYR:CD1	10:J:10:GLY:HA2	2.49	0.48
1:A:1240:U:OP2	7:G:116:ALA:N	2.46	0.48
1:A:1275:A:C2'	1:A:1276:G:H5'	2.43	0.48
1:A:1513:A:H2'	1:A:1514:C:C6	2.48	0.48
1:A:429:U:O3'	4:D:22:LYS:NZ	2.45	0.48
1:A:811:C:N4	30:A:4019:HOH:O	2.45	0.48
10:J:7:LYS:HB2	10:J:97:GLU:HB2	1.95	0.48
18:R:41:LYS:HE3	18:R:41:LYS:HB3	1.73	0.48
23:Y:29:G:N2	23:Y:41:C:N3	2.55	0.48
23:Y:65:G:H2'	23:Y:66:U:C6	2.48	0.48
1:A:1073:U:O2	2:B:104:ASN:ND2	2.38	0.48
7:G:90:GLU:CD	7:G:90:GLU:H	2.15	0.48
12:L:28:LYS:N	12:L:29:GLY:HA2	2.29	0.48
1:A:1033:G:H2'	1:A:1034:G:H8	1.78	0.48
1:A:1397:C:OP2	5:E:24:ARG:NH2	2.46	0.48
1:A:1292:U:P	7:G:41:ARG:HH22	2.37	0.48
5:E:93:PRO:HG2	8:H:105:ARG:NE	2.29	0.48
2:B:63:MET:HG3	2:B:225:ALA:HB1	1.95	0.48
1:A:1272:G:H2'	1:A:1273:G:O4'	2.14	0.47
1:A:659:U:C2'	1:A:660:G:H5'	2.44	0.47
3:C:149:ALA:HA	3:C:201:TYR:O	2.14	0.47
1:A:1016:A:H2'	1:A:1017:G:O4'	2.14	0.47
1:A:1069:C:O2'	1:A:1192:C:H1'	2.14	0.47
2:B:48:MET:O	2:B:52:GLU:N	2.44	0.47
3:C:174:PRO:HD2	3:C:182:ILE:HD11	1.96	0.47
23:Y:61:C:H2'	23:Y:62:C:C6	2.48	0.47
1:A:1142:G:H2'	1:A:1143:G:O4'	2.15	0.47
1:A:1162:C:N3	1:A:1174:G:N2	2.61	0.47
7:G:79:ARG:HG2	7:G:79:ARG:HH21	1.79	0.47
9:I:85:LEU:HD12	9:I:96:LEU:HD11	1.95	0.47
23:Y:55:PSU:HN1	23:Y:57:G:H5'	1.78	0.47
2:B:163:PHE:HA	2:B:185:ILE:HG12	1.96	0.47
20:T:14:LYS:O	20:T:18:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1273:G:H3'	1:A:1274:G:C8	2.49	0.47
1:A:1330:U:H4'	13:M:23:TYR:CE1	2.49	0.47
1:A:1519:A:H5''	1:A:1520:G:OP2	2.15	0.47
9:I:23:ASN:HD22	9:I:24:GLY:N	2.13	0.47
7:G:97:GLN:O	7:G:101:LEU:HG	2.15	0.47
16:P:8:ARG:HB3	16:P:28:ARG:NH1	2.30	0.47
23:W:3:C:N3	23:W:70:G:O6	2.47	0.47
23:W:7:A:H5'	23:W:8:4SU:H5	1.95	0.47
2:B:71:VAL:HG21	2:B:164:VAL:HG22	1.97	0.47
1:A:1194:U:H4'	5:E:22:GLY:HA3	1.96	0.47
8:H:51:VAL:HG12	8:H:52:ASP:H	1.79	0.47
1:A:1120:G:C6	1:A:1121:U:C4	3.03	0.47
3:C:152:ILE:HD12	3:C:199:LYS:HD2	1.95	0.47
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.95	0.47
4:D:173:TRP:CZ3	4:D:193:ASP:HB3	2.50	0.47
4:D:20:TYR:CD2	4:D:26:CYS:HB3	2.50	0.47
7:G:108:ALA:HA	7:G:111:ARG:HD2	1.97	0.47
17:Q:54:GLY:O	17:Q:81:ARG:N	2.41	0.47
19:S:27:GLU:HB3	19:S:28:LYS:HD3	1.97	0.47
9:I:128:ARG:HH21	24:X:32:5MC:P	2.38	0.47
1:A:7:G:H5'	1:A:298:A:O4'	2.14	0.47
13:M:84:ILE:HG13	13:M:85:GLY:N	2.29	0.47
5:E:24:ARG:NH1	22:V:24:A:OP2	2.48	0.47
1:A:1034:G:H3'	1:A:1035:A:H8	1.78	0.47
1:A:1178:G:N2	1:A:1180:A:H3'	2.30	0.47
1:A:520:A:N1	1:A:536:C:H1'	2.30	0.47
1:A:750:G:O2'	15:O:21:ASP:OD1	2.33	0.47
2:B:188:ALA:HB1	2:B:192:SER:OG	2.15	0.47
3:C:34:LEU:O	3:C:38:ARG:HB2	2.14	0.47
5:E:43:LEU:O	5:E:65:ASN:ND2	2.38	0.47
1:A:1318:A:H5''	19:S:3:ARG:NH2	2.30	0.47
1:A:1207:G:C6	1:A:1208:C:C4	3.03	0.46
1:A:1239:A:H62	1:A:1299:A:N6	2.12	0.46
1:A:664:G:N2	1:A:741:G:H1	2.11	0.46
1:A:19:C:H5''	5:E:86:ALA:HB3	1.97	0.46
22:V:23:A:H4'	22:V:24:A:C5'	2.42	0.46
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.98	0.46
1:A:707:C:OP1	11:K:85:ARG:NH1	2.48	0.46
23:Y:58:A:O2'	23:Y:60:U:OP2	2.31	0.46
1:A:1410:G:H2'	1:A:1411:C:H6	1.80	0.46
1:A:807:A:H2'	1:A:808:C:C6	2.51	0.46
2:B:118:LEU:HD13	2:B:142:LEU:HB2	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:16:HIS:CG	2:B:17:PHE:H	2.33	0.46
1:A:8:A:N6	4:D:209:ARG:HB2	2.31	0.46
10:J:50:ILE:HB	14:N:41:ARG:NH2	2.30	0.46
1:A:1001(A):G:H3'	1:A:1002:G:O4'	2.16	0.46
1:A:1002:G:H2'	1:A:1003:G:H8	1.81	0.46
1:A:1256:A:HO2'	1:A:1257:U:P	2.37	0.46
1:A:975:A:H5'	1:A:975:A:H8	1.81	0.46
3:C:102:ASN:N	3:C:102:ASN:HD22	2.13	0.46
3:C:125:GLU:O	3:C:127:ARG:NH1	2.45	0.46
1:A:972:C:O2'	10:J:55:LYS:O	2.27	0.46
1:A:444:C:H2'	1:A:445:G:H8	1.80	0.46
1:A:975:A:H4'	1:A:976:G:C5'	2.43	0.46
8:H:49:GLU:HG2	8:H:62:TYR:HE1	1.81	0.46
13:M:92:HIS:CE1	13:M:98:VAL:HG21	2.51	0.46
1:A:165:C:H2'	1:A:166:G:H8	1.80	0.46
1:A:392:G:H2'	1:A:393:A:C8	2.51	0.46
1:A:560:U:O2'	1:A:561:U:OP2	2.27	0.46
1:A:735:C:H2'	1:A:736:C:H6	1.80	0.46
1:A:828:A:H2'	1:A:829:G:O4'	2.16	0.46
7:G:32:ARG:HH12	7:G:109:ASN:ND2	2.12	0.46
10:J:8:LEU:HD12	10:J:20:ALA:HB2	1.97	0.46
20:T:60:GLU:HG3	20:T:81:LYS:HD2	1.98	0.46
23:W:51:U:O5'	23:W:51:U:H6	1.97	0.46
23:Y:8:4SU:O2	23:Y:21:A:H2	1.97	0.46
1:A:1122:U:C4	1:A:1123:A:N7	2.84	0.46
4:D:8:VAL:HG13	4:D:21:LEU:HD12	1.97	0.46
6:F:36:ARG:HH11	6:F:38:GLU:HG2	1.81	0.46
12:L:37:CYS:SG	12:L:81:SER:HB2	2.56	0.46
13:M:122:LYS:HD3	13:M:123:ALA:N	2.17	0.46
16:P:69:THR:HB	16:P:72:ARG:HH12	1.81	0.46
1:A:1032:G:H2'	1:A:1033:G:C8	2.51	0.46
1:A:1380:U:C4	7:G:3:ARG:HG2	2.50	0.46
3:C:137:ALA:HA	3:C:140:ARG:CZ	2.45	0.46
13:M:19:LEU:HD11	13:M:56:LEU:HD21	1.97	0.46
23:W:34:G:H2'	23:W:35:A:C8	2.51	0.46
1:A:1001(A):G:C4	1:A:1002:G:H1'	2.50	0.46
1:A:1105:A:H2'	1:A:1106:G:H8	1.81	0.46
1:A:841:U:C5	1:A:848:C:H1'	2.51	0.46
2:B:189:ASP:OD1	2:B:189:ASP:N	2.49	0.46
3:C:157:ILE:HD13	3:C:166:GLU:HG3	1.97	0.46
14:N:21:TYR:HE1	14:N:23:ARG:NE	2.14	0.46
16:P:22:THR:HA	16:P:33:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:53:VAL:O	16:P:57:ARG:HB2	2.16	0.46
23:Y:63:G:H2'	23:Y:64:A:O4'	2.16	0.46
1:A:1004:A:C2	1:A:1038:C:C4	3.04	0.46
1:A:1236:A:O2'	1:A:1304:G:H4'	2.16	0.46
1:A:142:G:H2'	1:A:143:A:C8	2.51	0.46
1:A:96:U:HO2'	1:A:97:G:H8	1.60	0.46
5:E:42:GLY:HA2	5:E:65:ASN:O	2.16	0.46
5:E:53:LEU:H	5:E:53:LEU:HD12	1.80	0.46
7:G:10:ARG:HA	7:G:10:ARG:HD2	1.56	0.46
1:A:1302:U:OP2	13:M:21:TYR:OH	2.13	0.45
23:Y:62:C:H2'	23:Y:63:G:H8	1.80	0.45
1:A:1039:C:C4	1:A:1040:U:C4	3.05	0.45
1:A:232:G:H1'	1:A:262:A:N1	2.31	0.45
1:A:833:U:H2'	1:A:834:C:C6	2.51	0.45
1:A:91:C:H2'	1:A:92:C:C6	2.51	0.45
1:A:992:U:H4'	1:A:993:G:O5'	2.16	0.45
2:B:88:ALA:HB1	2:B:90:MET:HG3	1.98	0.45
2:B:97:TRP:NE1	2:B:173:ALA:HB2	2.31	0.45
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.31	0.45
1:A:1392:G:N2	1:A:1502:A:H8	2.14	0.45
1:A:659:U:H2'	1:A:660:G:H5'	1.99	0.45
8:H:19:VAL:HG23	8:H:21:LYS:HG3	1.98	0.45
8:H:25:ASP:OD1	8:H:25:ASP:N	2.50	0.45
9:I:58:HIS:CD2	9:I:58:HIS:H	2.33	0.45
23:W:50:U:O2	23:W:64:A:N1	2.50	0.45
1:A:187:C:H2'	1:A:188:C:H6	1.82	0.45
1:A:728:A:OP1	1:A:742:G:O2'	2.34	0.45
2:B:78:GLN:O	2:B:94:ASN:ND2	2.49	0.45
7:G:77:SER:HA	7:G:85:TYR:O	2.16	0.45
12:L:60:LEU:HD11	12:L:85:ILE:HD13	1.98	0.45
20:T:50:GLU:O	20:T:100:ILE:HD11	2.15	0.45
1:A:1055:A:C5	1:A:1206:G:C2	3.05	0.45
1:A:109:A:C6	1:A:326:G:C6	3.05	0.45
1:A:154:C:C2'	1:A:155:C:H5'	2.47	0.45
26:A:3202:UAM:OAE	26:A:3202:UAM:NAD	2.49	0.45
5:E:13:ILE:O	5:E:13:ILE:HG13	2.16	0.45
1:A:955:U:O2'	19:S:83:HIS:HD2	2.00	0.45
1:A:1133:G:H1	1:A:1141:C:H42	1.65	0.45
1:A:1162:C:N4	1:A:1174:G:N1	2.63	0.45
1:A:509:A:H5''	4:D:55:ALA:HB2	1.98	0.45
15:O:18:PHE:CE2	15:O:21:ASP:HB2	2.51	0.45
23:Y:69:G:H2'	23:Y:70:G:O4'	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1134:G:C2'	1:A:1135:U:H5'	2.46	0.45
1:A:1291:G:C6	1:A:1292:U:C4	3.04	0.45
1:A:836:G:C6	1:A:851:G:C6	3.04	0.45
6:F:50:TYR:CE2	18:R:77:GLY:HA2	2.52	0.45
10:J:70:ARG:HA	10:J:70:ARG:HD3	1.84	0.45
19:S:27:GLU:HG2	19:S:47:HIS:NE2	2.32	0.45
19:S:80:TYR:CZ	19:S:82:GLY:HA2	2.51	0.45
23:Y:18:G:C2	23:Y:55:PSU:C4	3.05	0.45
1:A:1036:G:H2'	1:A:1037:C:O4'	2.17	0.45
1:A:1305:G:H5'	21:U:4:GLY:HA3	1.98	0.45
1:A:964:A:N3	1:A:969:A:O2'	2.36	0.45
1:A:408:A:H4'	4:D:112:VAL:HG21	1.99	0.45
5:E:100:VAL:HG22	5:E:118:ILE:HG22	1.99	0.45
10:J:27:ALA:HB1	10:J:74:ILE:HD13	1.98	0.45
3:C:8:ILE:HD13	3:C:184:TYR:HB3	1.99	0.45
1:A:1151:A:O4'	10:J:39:PRO:HB2	2.16	0.45
1:A:35:G:O2'	12:L:118:SER:O	2.25	0.45
12:L:32:PHE:HB3	12:L:84:LEU:HD11	1.99	0.45
17:Q:43:LEU:HG	17:Q:68:ARG:HH11	1.80	0.45
20:T:57:ARG:NH1	20:T:101:GLY:O	2.50	0.45
1:A:188:C:O4'	20:T:89:ARG:NH2	2.50	0.45
1:A:1004:A:H5''	1:A:1025:U:C5	2.52	0.45
1:A:1004:A:H3'	1:A:1005:A:C5'	2.47	0.45
1:A:1298:C:H2'	7:G:114:ARG:HH12	1.82	0.45
1:A:1469:G:H2'	1:A:1470:G:C8	2.52	0.45
2:B:53:ARG:O	2:B:56:ARG:HB3	2.17	0.45
3:C:148:GLY:HA3	3:C:172:ARG:O	2.17	0.45
3:C:7:PRO:O	3:C:11:ARG:NH1	2.46	0.45
5:E:33:VAL:HG13	5:E:112:LEU:HD12	1.98	0.45
6:F:82:ARG:HD2	6:F:82:ARG:HA	1.66	0.45
7:G:38:LEU:O	7:G:42:ILE:HG13	2.17	0.45
20:T:43:LEU:HD12	20:T:55:ILE:HG13	1.98	0.45
23:Y:59:U:H3'	23:Y:60:U:O2	2.17	0.45
1:A:1080:A:H5''	1:A:1081:G:OP2	2.17	0.44
1:A:142:G:H2'	1:A:143:A:H8	1.82	0.44
1:A:162:A:O5'	1:A:162:A:H8	2.00	0.44
2:B:97:TRP:CZ2	2:B:173:ALA:HA	2.52	0.44
18:R:53:ARG:HH21	18:R:59:SER:HA	1.82	0.44
24:X:21:A:N6	24:X:46:G:H2'	2.32	0.44
1:A:987:G:H1	1:A:1218:C:H42	1.65	0.44
1:A:1246:C:H2'	1:A:1247:U:C6	2.53	0.44
1:A:580:U:H2'	1:A:581:G:O4'	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:651:C:N4	1:A:753:A:OP2	2.50	0.44
20:T:16:HIS:O	20:T:19:SER:OG	2.26	0.44
23:Y:19:G:N1	23:Y:56:C:C4	2.85	0.44
1:A:1001(A):G:C5	1:A:1002:G:H1'	2.52	0.44
1:A:1251:A:N1	1:A:1354:C:O2'	2.42	0.44
1:A:1262:C:H2'	1:A:1263:C:C6	2.53	0.44
1:A:371:G:H1'	1:A:482:A:H1'	2.00	0.44
9:I:23:ASN:HD22	9:I:24:GLY:H	1.64	0.44
9:I:37:PHE:HD1	9:I:40:LEU:HD12	1.82	0.44
23:W:61:C:O2'	23:W:62:C:O4'	2.36	0.44
1:A:1261:A:H3'	1:A:1262:C:C6	2.52	0.44
2:B:111:ARG:HD3	2:B:111:ARG:HA	1.71	0.44
2:B:185:ILE:HG22	2:B:199:TYR:HB2	1.99	0.44
5:E:144:THR:O	5:E:148:VAL:HG23	2.18	0.44
5:E:79:GLU:N	5:E:79:GLU:OE1	2.38	0.44
23:W:4:C:N3	23:W:69:G:C2	2.85	0.44
24:X:19:G:H4'	24:X:20:U:OP2	2.16	0.44
23:Y:2:C:H2'	23:Y:3:C:C6	2.52	0.44
1:A:1022:G:H2'	1:A:1023:G:C8	2.53	0.44
1:A:1095:U:OP1	1:A:1108:G:N2	2.44	0.44
5:E:76:ILE:O	5:E:93:PRO:HB3	2.17	0.44
20:T:77:ALA:O	20:T:81:LYS:HG3	2.18	0.44
24:X:31:G:C8	24:X:32:5MC:HM52	2.53	0.44
1:A:1245:A:H61	1:A:1292:U:H3	1.66	0.44
1:A:920:U:H2'	1:A:921:U:H6	1.82	0.44
1:A:952:U:O4	13:M:104:ARG:HD3	2.17	0.44
2:B:197:VAL:HB	2:B:200:ILE:HG23	2.00	0.44
2:B:213:LEU:O	2:B:217:ARG:HB2	2.17	0.44
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.50	0.44
23:Y:21:A:N6	23:Y:46:7MG:H1'	2.32	0.44
1:A:583:A:H2'	1:A:584:G:O4'	2.17	0.44
1:A:977:A:O2'	1:A:981:U:N3	2.45	0.44
1:A:983:A:H2	1:A:984:C:C6	2.36	0.44
1:A:986:A:H2'	1:A:987:G:O4'	2.16	0.44
10:J:48:THR:OG1	10:J:62:HIS:ND1	2.46	0.44
11:K:80:VAL:HG13	11:K:103:LEU:HD12	1.98	0.44
18:R:45:SER:OG	18:R:47:THR:HG22	2.18	0.44
18:R:76:LEU:HD12	18:R:76:LEU:HA	1.77	0.44
18:R:84:LYS:H	18:R:84:LYS:HG2	1.53	0.44
24:X:23:C:H2'	24:X:24:U:C6	2.53	0.44
1:A:1316:G:O2'	1:A:1318:A:N7	2.48	0.44
3:C:36:ASP:O	3:C:40:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:47:ARG:O	4:D:47:ARG:HD3	2.18	0.44
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.99	0.44
10:J:49:VAL:HG21	14:N:41:ARG:O	2.18	0.44
3:C:22:TRP:CZ2	14:N:54:PRO:HG3	2.53	0.44
1:A:109:A:H5'	1:A:110:C:C5	2.53	0.44
1:A:1157:A:H4'	1:A:1158:C:O5'	2.18	0.44
1:A:748:C:H4'	1:A:749:C:O5'	2.18	0.44
5:E:78:HIS:HA	8:H:105:ARG:HG3	2.00	0.44
8:H:82:HIS:HE2	8:H:84:ARG:HG2	1.83	0.44
17:Q:27:PHE:CE2	17:Q:36:ILE:HD11	2.53	0.44
23:Y:9:A:O2'	23:Y:11:C:N4	2.45	0.44
1:A:1117:G:N2	1:A:1180:A:H1'	2.31	0.43
1:A:1236:A:H2'	1:A:1237:C:C6	2.53	0.43
1:A:833:U:H2'	1:A:834:C:H6	1.82	0.43
2:B:55:PHE:CE1	2:B:218:ALA:HA	2.53	0.43
3:C:175:LEU:HD21	3:C:201:TYR:CE1	2.53	0.43
4:D:155:LEU:O	4:D:159:ARG:HG3	2.17	0.43
9:I:11:LYS:HA	9:I:108:VAL:HG13	1.99	0.43
16:P:40:ASP:O	16:P:48:TRP:HB2	2.18	0.43
1:A:1424:C:H2'	1:A:1425:U:O4'	2.18	0.43
3:C:131:ARG:HH11	5:E:50:GLU:HG3	1.83	0.43
9:I:102:LEU:HD13	9:I:103:THR:N	2.28	0.43
10:J:16:LEU:HD12	10:J:70:ARG:HG2	1.99	0.43
13:M:96:LEU:O	13:M:110:ARG:NH1	2.50	0.43
18:R:58:LEU:HD12	18:R:62:GLU:HB2	2.00	0.43
1:A:1134:G:H2'	1:A:1134:G:N3	2.34	0.43
1:A:1441:G:O5'	1:A:1441:G:H8	2.02	0.43
1:A:340:U:H2'	1:A:341:C:C6	2.53	0.43
4:D:11:LEU:O	4:D:15:GLU:HG2	2.18	0.43
9:I:50:LEU:H	9:I:50:LEU:HG	1.46	0.43
1:A:689:C:P	11:K:46:GLY:HA3	2.59	0.43
20:T:50:GLU:HB2	20:T:99:LEU:CD2	2.47	0.43
1:A:1159:U:H5''	1:A:1182:G:H21	1.83	0.43
1:A:1316:G:N1	1:A:1319:A:OP2	2.49	0.43
1:A:179:A:H2'	1:A:180:U:C6	2.54	0.43
1:A:959:A:O2'	1:A:984:C:O2'	2.33	0.43
2:B:101:MET:HA	2:B:108:ILE:HG12	2.00	0.43
8:H:33:GLU:HG2	8:H:48:TYR:CE2	2.53	0.43
10:J:10:GLY:HA3	10:J:16:LEU:HD21	2.01	0.43
19:S:36:ARG:HD2	19:S:52:TYR:O	2.19	0.43
1:A:1133:G:C4	1:A:1134:G:C8	3.07	0.43
1:A:1368:G:OP1	9:I:111:ARG:NH2	2.35	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:187:C:H2'	1:A:188:C:C6	2.53	0.43
1:A:769:G:H4'	1:A:1513:A:H4'	2.01	0.43
2:B:105:PHE:CE1	2:B:155:LEU:HD12	2.53	0.43
2:B:12:GLU:HA	2:B:15:VAL:HG23	2.01	0.43
2:B:19:HIS:CG	2:B:20:GLU:H	2.37	0.43
12:L:24:VAL:HB	12:L:27:LEU:HD22	1.98	0.43
1:A:523:A:H61	12:L:92:ASP:HB2	1.83	0.43
16:P:57:ARG:HH21	16:P:79:VAL:HA	1.83	0.43
19:S:12:ASP:OD1	19:S:37:ARG:NH1	2.51	0.43
23:W:39:PSU:H2'	23:W:40:C:C6	2.53	0.43
23:W:40:C:H2'	23:W:41:C:H6	1.82	0.43
1:A:1144:G:N2	1:A:1146:A:H62	2.16	0.43
1:A:1119:C:N4	1:A:1154:G:H1	2.13	0.43
1:A:299:G:H2'	1:A:300:A:C8	2.53	0.43
26:A:3202:UAM:OAG	26:A:3202:UAM:OAH	2.32	0.43
1:A:643:C:H2'	1:A:644:G:H8	1.84	0.43
4:D:180:GLY:O	4:D:182:LYS:HD3	2.18	0.43
4:D:196:LEU:H	4:D:196:LEU:HD12	1.83	0.43
8:H:6:ILE:O	8:H:10:LEU:HG	2.18	0.43
23:Y:19:G:N2	23:Y:56:C:C2	2.83	0.43
1:A:1020:U:C2	1:A:1021:G:C8	3.07	0.43
1:A:1066:C:C2'	1:A:1067:A:H5'	2.49	0.43
2:B:17:PHE:HA	2:B:44:LEU:HD11	1.99	0.43
4:D:3:ARG:O	4:D:5:ILE:HG22	2.18	0.43
5:E:33:VAL:HG21	5:E:109:ILE:HA	2.00	0.43
7:G:20:ASP:OD1	7:G:22:LEU:HB3	2.19	0.43
15:O:62:GLN:O	15:O:66:LEU:HD13	2.19	0.43
16:P:74:LEU:O	16:P:79:VAL:HG23	2.19	0.43
1:A:1064:G:H4'	1:A:1065:U:O5'	2.19	0.43
1:A:1095:U:H2'	1:A:1096:C:C6	2.54	0.43
1:A:1162:C:C2	1:A:1174:G:N2	2.86	0.43
1:A:1375:A:H4'	7:G:29:LYS:HD3	1.99	0.43
1:A:539:A:H2'	1:A:540:G:C8	2.53	0.43
2:B:80:ILE:HD11	2:B:212:GLN:CA	2.48	0.43
1:A:376:G:H4'	16:P:5:ARG:HD3	2.01	0.43
1:A:1132:C:N3	1:A:1142:G:N2	2.61	0.43
1:A:620:C:H2'	1:A:621:A:O4'	2.19	0.43
2:B:185:ILE:HG22	2:B:199:TYR:CD2	2.51	0.43
1:A:619:U:N3	4:D:134:ASP:OD1	2.46	0.43
1:A:7:G:O2'	5:E:120:THR:O	2.36	0.43
23:W:67:C:H2'	23:W:68:C:C6	2.54	0.43
22:V:14:A:C6	23:Y:34:G:C5	3.06	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1084:G:H5'	1:A:1102:A:OP2	2.19	0.43
1:A:1516:G:H2'	1:A:1518:A:OP2	2.19	0.43
1:A:701:C:OP1	1:A:702:A:O2'	2.21	0.43
1:A:545:C:OP2	4:D:65:ARG:NH2	2.52	0.43
5:E:113:ALA:HB3	5:E:115:VAL:HG23	2.01	0.43
5:E:13:ILE:HA	5:E:29:GLY:O	2.19	0.43
7:G:100:ALA:O	7:G:104:LEU:HB2	2.18	0.43
8:H:64:LYS:HB3	8:H:79:VAL:HG21	2.01	0.43
17:Q:45:HIS:CD2	17:Q:47:PRO:HD3	2.54	0.43
1:A:194:C:H2'	1:A:195:A:H5''	2.00	0.42
1:A:524:G:H2'	1:A:525:C:C6	2.53	0.42
1:A:78:G:C2'	1:A:79:G:H5'	2.49	0.42
9:I:4:TYR:CE2	9:I:88:TYR:HA	2.54	0.42
13:M:108:ARG:HD3	13:M:108:ARG:HA	1.74	0.42
18:R:53:ARG:HA	18:R:56:THR:OG1	2.19	0.42
1:A:1220:G:N2	19:S:54:GLY:O	2.50	0.42
23:W:6:G:O6	23:W:67:C:N3	2.52	0.42
1:A:1023:G:H3'	1:A:1024:G:H8	1.84	0.42
1:A:1228:C:H2'	1:A:1229:A:H8	1.83	0.42
1:A:255:G:C6	1:A:256:U:C4	3.08	0.42
1:A:662:G:O2'	1:A:836:G:OP1	2.33	0.42
2:B:16:HIS:HB3	2:B:210:SER:HB2	2.01	0.42
8:H:13:ILE:O	8:H:17:THR:HG23	2.19	0.42
9:I:7:THR:HB	9:I:83:ARG:NH1	2.34	0.42
14:N:6:LEU:HB3	14:N:23:ARG:NH2	2.35	0.42
16:P:3:LYS:O	16:P:21:VAL:HA	2.19	0.42
23:W:8:4SU:H1'	23:W:48:C:H1'	2.01	0.42
23:Y:46:7MG:H2'	23:Y:46:7MG:H82	1.74	0.42
23:Y:68:C:H2'	23:Y:69:G:H5'	2.01	0.42
23:Y:8:4SU:S4	23:Y:14:A:N7	2.92	0.42
1:A:1012:U:O2	1:A:1017:G:O6	2.37	0.42
1:A:1135:U:H4'	1:A:1136:U:H5	1.84	0.42
1:A:991:U:O2'	1:A:1212:U:C4	2.71	0.42
1:A:1222:G:OP1	19:S:77:THR:HG21	2.19	0.42
1:A:457:C:H2'	1:A:458:C:C6	2.53	0.42
1:A:69:G:H2'	1:A:70:G:H8	1.84	0.42
2:B:210:SER:OG	2:B:211:ILE:N	2.51	0.42
9:I:48:GLU:O	9:I:51:ARG:HB2	2.19	0.42
12:L:39:VAL:HG11	12:L:41:ARG:HH11	1.84	0.42
23:Y:51:U:O2	23:Y:63:G:N2	2.40	0.42
1:A:1009:G:H22	1:A:1021:G:H1'	1.85	0.42
1:A:1009:G:C2	1:A:1021:G:N3	2.87	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:153:C:H2'	1:A:154:C:C6	2.55	0.42
2:B:47:THR:HA	2:B:202:PRO:CG	2.46	0.42
4:D:173:TRP:CD1	4:D:174:LEU:HG	2.55	0.42
4:D:153:ARG:HD3	4:D:181:MET:CE	2.50	0.42
13:M:4:ILE:HG23	13:M:5:ALA:N	2.30	0.42
17:Q:26:GLN:HG2	17:Q:37:LYS:HG2	2.01	0.42
1:A:300:A:H1'	1:A:565:U:O2	2.19	0.42
1:A:664:G:P	18:R:64:ARG:HH21	2.41	0.42
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.59	0.42
5:E:105:VAL:HB	5:E:106:PRO:HD3	2.01	0.42
15:O:29:VAL:HG13	15:O:63:ARG:HG3	2.01	0.42
19:S:48:THR:HA	19:S:60:VAL:O	2.19	0.42
1:A:1286:A:H8	1:A:1287:A:H4'	1.83	0.42
1:A:391:G:C6	1:A:392:G:C5	3.07	0.42
1:A:683:G:O6	30:A:4140:HOH:O	2.19	0.42
20:T:87:LYS:O	20:T:91:LEU:HG	2.19	0.42
24:X:20:U:H5''	24:X:21:A:OP2	2.19	0.42
1:A:942:G:C2	1:A:1342:C:C2	3.08	0.42
1:A:1410:G:H2'	1:A:1411:C:C6	2.55	0.42
1:A:337:C:H2'	1:A:338:A:C8	2.55	0.42
1:A:26:A:N6	1:A:558:G:O2'	2.48	0.42
1:A:978:A:H1'	1:A:1322:C:O2	2.20	0.42
13:M:60:VAL:HG22	13:M:66:LEU:HD11	2.01	0.42
23:Y:55:PSU:HN1	23:Y:57:G:C5'	2.32	0.42
1:A:1013:G:O2'	1:A:1015:A:N7	2.52	0.42
1:A:1027:C:O2'	1:A:1034:G:N2	2.53	0.42
1:A:1510:U:H2'	1:A:1511:G:C8	2.55	0.42
2:B:15:VAL:HB	2:B:16:HIS:CD2	2.54	0.42
9:I:55:ALA:HA	9:I:58:HIS:CD2	2.54	0.42
1:A:881:G:OP2	12:L:12:ARG:NH2	2.52	0.42
20:T:90:GLN:HB2	20:T:90:GLN:HE21	1.58	0.42
1:A:110:C:H2'	1:A:111:G:O4'	2.20	0.42
1:A:1250:A:N3	1:A:1370:G:O2'	2.41	0.42
1:A:857:C:H2'	1:A:858:G:O4'	2.20	0.42
2:B:69:LEU:HD13	2:B:91:PRO:HB2	2.02	0.42
7:G:137:LYS:O	7:G:141:VAL:HG23	2.20	0.42
12:L:51:ALA:O	12:L:52:LEU:HD13	2.19	0.42
1:A:636:U:H5'	17:Q:2:PRO:HD3	2.02	0.42
17:Q:74:LEU:HD13	17:Q:75:ARG:HG2	2.01	0.42
1:A:1063:C:OP2	1:A:1064:G:O2'	2.29	0.42
1:A:1112:C:H1'	3:C:179:ARG:HG2	2.02	0.42
1:A:1323:G:H2'	1:A:1324:A:C8	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1287:A:H2	1:A:1353:G:H1'	1.85	0.42
1:A:1366:C:H2'	1:A:1367:C:C6	2.54	0.42
1:A:779:C:H2'	1:A:780:A:O4'	2.19	0.42
2:B:16:HIS:HB3	2:B:210:SER:HB3	2.02	0.42
4:D:121:VAL:O	4:D:134:ASP:HA	2.20	0.42
8:H:82:HIS:HB3	8:H:138:TRP:CE2	2.55	0.42
8:H:14:ARG:CG	8:H:18:ARG:HH22	2.32	0.42
23:W:49:C:H6	23:W:49:C:O5'	2.03	0.42
1:A:1035:A:H8	1:A:1035:A:O5'	2.02	0.41
1:A:1146:A:H5'	1:A:1146:A:H8	1.85	0.41
1:A:1476:G:H2'	1:A:1477:C:C6	2.55	0.41
1:A:735:C:H2'	1:A:736:C:C6	2.55	0.41
1:A:825:G:H1	1:A:875:C:H42	1.67	0.41
11:K:120:ARG:HA	11:K:121:PRO:HD3	1.89	0.41
17:Q:81:ARG:NH2	17:Q:84:LEU:HD21	2.35	0.41
1:A:1038:C:C2'	1:A:1039:C:H5'	2.50	0.41
1:A:1086:U:H3	1:A:1099:G:N2	2.17	0.41
1:A:1391:U:H2'	1:A:1392:G:C8	2.55	0.41
1:A:266:G:H5''	1:A:268:C:H41	1.85	0.41
3:C:33:LEU:HA	3:C:36:ASP:HB2	2.03	0.41
5:E:79:GLU:OE1	8:H:104:ARG:HA	2.20	0.41
1:A:671:G:H5'	6:F:77:ARG:HH22	1.85	0.41
13:M:13:LYS:NZ	13:M:21:TYR:OH	2.54	0.41
1:A:316:G:OP2	1:A:351:G:O2'	2.31	0.41
1:A:900:A:H2'	1:A:901:A:C8	2.56	0.41
22:V:12:A:OP2	22:V:12:A:H8	2.03	0.41
2:B:158:LEU:HA	2:B:159:PRO:HD3	1.88	0.41
3:C:152:ILE:CD1	3:C:199:LYS:HD2	2.50	0.41
7:G:51:GLN:HB3	7:G:51:GLN:HE21	1.62	0.41
1:A:589:C:H5''	8:H:29:SER:OG	2.20	0.41
13:M:88:ARG:HG3	13:M:98:VAL:CG1	2.48	0.41
21:U:5:ASP:O	21:U:11:GLY:HA3	2.20	0.41
1:A:1243:C:H42	1:A:1294:G:H1	1.68	0.41
1:A:353:A:H5'	1:A:353:A:C8	2.55	0.41
1:A:695:A:C6	1:A:696:A:C6	3.09	0.41
4:D:119:GLN:HG2	4:D:123:HIS:CD2	2.55	0.41
1:A:411:A:OP2	4:D:30:LYS:HE3	2.20	0.41
5:E:127:ASN:HA	5:E:128:PRO:HD3	1.89	0.41
7:G:22:LEU:HG	7:G:62:PHE:CE2	2.56	0.41
23:W:34:G:H2'	23:W:35:A:H8	1.85	0.41
1:A:1245:A:H2'	1:A:1246:C:O4'	2.21	0.41
1:A:714:G:H2'	1:A:715:A:C8	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:214:ILE:H	2:B:214:ILE:HG12	1.70	0.41
2:B:215:LEU:HA	2:B:215:LEU:HD22	1.94	0.41
7:G:50:ILE:HG22	7:G:125:MET:HG3	2.01	0.41
17:Q:62:SER:OG	17:Q:72:ARG:HD3	2.21	0.41
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.21	0.41
1:A:9:G:H2'	1:A:10:A:H8	1.85	0.41
1:A:1392:G:N2	1:A:1502:A:C8	2.89	0.41
1:A:407:G:H2'	1:A:408:A:C8	2.55	0.41
1:A:1060:C:C4	3:C:2:GLY:HA2	2.56	0.41
7:G:47:CYS:HA	7:G:50:ILE:HD11	2.03	0.41
7:G:52:GLU:H	7:G:52:GLU:HG2	1.45	0.41
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.35	0.41
20:T:51:GLU:O	20:T:55:ILE:HG12	2.20	0.41
1:A:1423:G:C6	1:A:1424:C:C4	3.09	0.41
1:A:854:G:C2	1:A:855:G:C8	3.09	0.41
1:A:865:A:H5'	1:A:1078:U:C5	2.56	0.41
4:D:173:TRP:CD1	4:D:189:PRO:HG3	2.55	0.41
6:F:95:GLU:HA	6:F:96:PRO:HD3	1.87	0.41
7:G:65:ALA:HB1	7:G:127:ALA:HB3	2.02	0.41
10:J:16:LEU:HA	10:J:16:LEU:HD22	1.84	0.41
1:A:1060:C:C5'	10:J:51:ARG:HB3	2.51	0.41
1:A:719:C:O2'	18:R:49:LYS:HB3	2.20	0.41
18:R:40:LEU:HB3	18:R:79:LEU:HD11	2.02	0.41
1:A:1191:A:H5''	3:C:4:LYS:HD3	2.02	0.41
2:B:28:PHE:O	2:B:32:ILE:HG13	2.20	0.41
3:C:63:ASN:HB3	3:C:98:ASN:HD22	1.86	0.41
8:H:97:VAL:HG23	8:H:129:VAL:O	2.21	0.41
9:I:7:THR:HB	9:I:83:ARG:HH12	1.85	0.41
3:C:126:ARG:HB3	3:C:128:PHE:CE1	2.56	0.41
8:H:121:ASP:OD1	8:H:121:ASP:N	2.53	0.41
1:A:1027:C:H5'	1:A:1028:C:OP2	2.21	0.41
1:A:1032:G:C2	1:A:1033:G:C5	3.09	0.41
1:A:685:G:C2	1:A:686:U:C4	3.09	0.41
1:A:765:G:H5''	1:A:766:A:OP1	2.21	0.41
1:A:839:U:O3'	1:A:840:C:H6	2.04	0.41
3:C:32:LEU:HD13	3:C:32:LEU:HA	1.90	0.41
5:E:51:VAL:O	5:E:55:VAL:HG23	2.20	0.41
5:E:84:PHE:N	5:E:87:SER:O	2.53	0.41
9:I:3:GLN:HG3	9:I:20:ARG:HE	1.86	0.41
10:J:23:ILE:HA	10:J:23:ILE:HD13	1.87	0.41
1:A:1228:C:P	13:M:108:ARG:HH22	2.39	0.41
1:A:1179:A:H5''	9:I:102:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1326:C:H2'	1:A:1327:C:C6	2.56	0.40
1:A:219:C:H2'	1:A:220:G:O4'	2.22	0.40
1:A:360:A:C6	1:A:361:G:C6	3.08	0.40
1:A:540:G:H2'	1:A:541:G:O4'	2.21	0.40
1:A:682:G:N7	30:A:4142:HOH:O	2.37	0.40
1:A:985:C:H2'	1:A:986:A:C8	2.56	0.40
3:C:119:ARG:O	3:C:123:GLN:HG3	2.21	0.40
15:O:69:TYR:CZ	15:O:73:GLU:HG3	2.56	0.40
23:Y:9:A:C2'	23:Y:11:C:H41	2.34	0.40
1:A:1190:G:HO2'	1:A:1191:A:P	2.45	0.40
1:A:390:C:H2'	1:A:391:G:C8	2.56	0.40
1:A:593:G:H2'	1:A:594:G:O4'	2.22	0.40
1:A:731:G:OP1	1:A:766:A:H1'	2.21	0.40
1:A:93:G:C6	1:A:96:U:C4	3.10	0.40
2:B:97:TRP:HE1	2:B:173:ALA:HB2	1.86	0.40
3:C:131:ARG:NE	3:C:166:GLU:OE2	2.54	0.40
12:L:54:LYS:HG2	12:L:75:HIS:CD2	2.56	0.40
12:L:88:GLY:O	12:L:99:HIS:HD2	2.04	0.40
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.56	0.40
18:R:33:ASP:OD2	18:R:36:ASN:HB2	2.22	0.40
18:R:44:LEU:HD23	18:R:50:ILE:HA	2.03	0.40
24:X:17:C:H2'	24:X:17(A):U:C5	2.56	0.40
23:Y:9:A:H8	23:Y:11:C:N4	2.19	0.40
1:A:126:G:H4'	1:A:634:C:O2	2.21	0.40
1:A:1305:G:O2'	1:A:1331:G:N2	2.53	0.40
1:A:1325:C:O2'	1:A:1326:C:H5'	2.21	0.40
1:A:811:C:H4'	1:A:900:A:N6	2.35	0.40
1:A:952:U:H2'	1:A:953:G:H8	1.86	0.40
2:B:77:ALA:HA	2:B:80:ILE:CG2	2.51	0.40
18:R:33:ASP:CG	18:R:36:ASN:HB2	2.42	0.40
19:S:12:ASP:OD2	19:S:14:HIS:NE2	2.55	0.40
1:A:1004:A:H2'	1:A:1038:C:H1'	2.03	0.40
1:A:1327:C:O2'	1:A:1328:C:H5'	2.21	0.40
1:A:266:G:H2'	1:A:266:G:H8	1.71	0.40
1:A:943:U:H2'	1:A:944:G:H5'	2.02	0.40
3:C:164:ARG:HG2	3:C:165:THR:H	1.86	0.40
7:G:125:MET:HE2	30:G:5101:HOH:O	2.20	0.40
7:G:50:ILE:HD11	7:G:58:PRO:HB3	2.03	0.40
2:B:179:LYS:HA	8:H:72:PRO:HG3	2.04	0.40
13:M:84:ILE:HG22	19:S:65:ASN:HB2	2.04	0.40
1:A:1032:G:OP2	1:A:1032:G:H8	2.04	0.40
1:A:1051:C:H2'	1:A:1052:U:H6	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1119:C:OP1	9:I:83:ARG:NH2	2.54	0.40
2:B:49:GLU:O	2:B:52:GLU:HB3	2.21	0.40
24:X:5:G:H1	24:X:68:C:N4	2.18	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	229/256 (90%)	201 (88%)	16 (7%)	12 (5%)	3	1
3	C	204/239 (85%)	188 (92%)	13 (6%)	3 (2%)	15	20
4	D	206/209 (99%)	201 (98%)	5 (2%)	0	100	100
5	E	146/162 (90%)	140 (96%)	5 (3%)	1 (1%)	30	43
6	F	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
7	G	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	18	24
8	H	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	I	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	27	39
10	J	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	11	12
11	K	112/129 (87%)	108 (96%)	2 (2%)	2 (2%)	13	15
12	L	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
13	M	120/126 (95%)	114 (95%)	4 (3%)	2 (2%)	14	17
14	N	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	O	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	19	26
16	P	80/88 (91%)	78 (98%)	1 (1%)	1 (1%)	18	24
17	Q	97/105 (92%)	96 (99%)	1 (1%)	0	100	100
18	R	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	S	81/93 (87%)	74 (91%)	6 (7%)	1 (1%)	19	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	94/106 (89%)	87 (93%)	2 (2%)	5 (5%)	3	1
21	U	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	2325/2538 (92%)	2192 (94%)	100 (4%)	33 (1%)	16	22

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	LEU
2	B	16	HIS
2	B	20	GLU
2	B	21	ARG
2	B	121	LEU
2	B	126	GLU
7	G	80	VAL
9	I	54	ASP
13	M	5	ALA
20	T	10	LEU
20	T	95	ALA
2	B	8	LYS
2	B	17	PHE
2	B	234	PRO
7	G	7	ALA
3	C	181	ASN
10	J	78	ASN
11	K	49	GLY
16	P	53	VAL
20	T	99	LEU
20	T	102	GLY
2	B	123	ALA
3	C	91	LEU
10	J	77	PRO
11	K	105	VAL
15	O	88	ARG
20	T	100	ILE
2	B	128	GLU
2	B	231	GLU
19	S	29	ARG
5	E	69	VAL
3	C	108	ASN
13	M	4	ILE

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	187/220 (85%)	158 (84%)	29 (16%)	4	4
3	C	140/188 (74%)	125 (89%)	15 (11%)	10	13
4	D	173/181 (96%)	158 (91%)	15 (9%)	15	22
5	E	114/123 (93%)	101 (89%)	13 (11%)	8	11
6	F	85/90 (94%)	77 (91%)	8 (9%)	13	18
7	G	120/127 (94%)	102 (85%)	18 (15%)	4	5
8	H	114/119 (96%)	100 (88%)	14 (12%)	7	8
9	I	89/99 (90%)	74 (83%)	15 (17%)	3	3
10	J	69/92 (75%)	64 (93%)	5 (7%)	21	31
11	K	83/99 (84%)	81 (98%)	2 (2%)	61	81
12	L	97/109 (89%)	92 (95%)	5 (5%)	32	49
13	M	92/101 (91%)	80 (87%)	12 (13%)	6	7
14	N	49/50 (98%)	39 (80%)	10 (20%)	2	2
15	O	78/80 (98%)	68 (87%)	10 (13%)	6	7
16	P	68/74 (92%)	63 (93%)	5 (7%)	20	30
17	Q	94/97 (97%)	88 (94%)	6 (6%)	25	37
18	R	59/77 (77%)	54 (92%)	5 (8%)	15	23
19	S	67/80 (84%)	61 (91%)	6 (9%)	14	20
20	T	70/82 (85%)	63 (90%)	7 (10%)	11	16
21	U	18/22 (82%)	15 (83%)	3 (17%)	3	3
All	All	1866/2110 (88%)	1663 (89%)	203 (11%)	9	13

All (203) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	10	LEU
2	B	15	VAL

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Mol	Chain	Res	Type
2	B	23	ARG
2	B	24	TRP
2	B	28	PHE
2	B	48	MET
2	B	71	VAL
2	B	76	GLN
2	B	81	VAL
2	B	87	ARG
2	B	94	ASN
2	B	96	ARG
2	B	97	TRP
2	B	115	LEU
2	B	124	SER
2	B	126	GLU
2	B	127	ILE
2	B	155	LEU
2	B	157	ARG
2	B	163	PHE
2	B	185	ILE
2	B	187	LEU
2	B	195	ASP
2	B	200	ILE
2	B	215	LEU
2	B	217	ARG
2	B	222	ILE
3	C	3	ASN
3	C	8	ILE
3	C	15	THR
3	C	36	ASP
3	C	45	LYS
3	C	54	ARG
3	C	70	VAL
3	C	85	ARG
3	C	102	ASN
3	C	104	GLN
3	C	108	ASN
3	C	115	LEU
3	C	131	ARG
3	C	152	ILE
3	C	196	LEU
4	D	8	VAL
4	D	19	LEU

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Mol	Chain	Res	Type
4	D	31	CYS
4	D	34	GLU
4	D	47	ARG
4	D	58	LEU
4	D	61	LYS
4	D	108	LEU
4	D	135	LEU
4	D	141	ARG
4	D	150	GLU
4	D	157	LEU
4	D	170	VAL
4	D	182	LYS
4	D	194	LEU
5	E	13	ILE
5	E	24	ARG
5	E	31	LEU
5	E	38	GLN
5	E	41	VAL
5	E	47	LYS
5	E	51	VAL
5	E	57	LYS
5	E	60	TYR
5	E	71	LEU
5	E	78	HIS
5	E	79	GLU
5	E	150	ARG
6	F	21	LEU
6	F	28	ARG
6	F	41	GLU
6	F	69	GLU
6	F	70	ASP
6	F	74	ASP
6	F	75	LEU
6	F	82	ARG
7	G	9	VAL
7	G	10	ARG
7	G	13	GLN
7	G	31	MET
7	G	41	ARG
7	G	51	GLN
7	G	52	GLU
7	G	73	MET

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Mol	Chain	Res	Type
7	G	76	ARG
7	G	78	ARG
7	G	79	ARG
7	G	90	GLU
7	G	98	SER
7	G	104	LEU
7	G	113	GLU
7	G	114	ARG
7	G	136	LYS
7	G	155	ARG
8	H	23	SER
8	H	25	ASP
8	H	29	SER
8	H	42	GLU
8	H	51	VAL
8	H	52	ASP
8	H	63	LEU
8	H	68	ARG
8	H	78	GLN
8	H	84	ARG
8	H	97	VAL
8	H	98	LYS
8	H	112	LEU
8	H	127	LEU
9	I	3	GLN
9	I	23	ASN
9	I	27	THR
9	I	42	ARG
9	I	50	LEU
9	I	56	LEU
9	I	65	VAL
9	I	81	ILE
9	I	83	ARG
9	I	89	ASN
9	I	102	LEU
9	I	108	VAL
9	I	112	LYS
9	I	121	ARG
9	I	128	ARG
10	J	9	ARG
10	J	16	LEU
10	J	21	GLN

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Mol	Chain	Res	Type
10	J	33	GLN
10	J	70	ARG
11	K	54	ARG
11	K	103	LEU
12	L	18	VAL
12	L	33	ARG
12	L	37	CYS
12	L	53	ARG
12	L	83	VAL
13	M	11	ARG
13	M	15	VAL
13	M	17	VAL
13	M	19	LEU
13	M	32	GLU
13	M	34	LEU
13	M	48	LEU
13	M	50	GLU
13	M	98	VAL
13	M	110	ARG
13	M	117	VAL
13	M	121	LYS
14	N	3	ARG
14	N	6	LEU
14	N	7	ILE
14	N	12	ARG
14	N	22	THR
14	N	23	ARG
14	N	29	ARG
14	N	33	VAL
14	N	41	ARG
14	N	44	LEU
15	O	3	ILE
15	O	5	LYS
15	O	10	LYS
15	O	26	GLU
15	O	38	ARG
15	O	39	LEU
15	O	41	GLU
15	O	54	ARG
15	O	71	GLN
15	O	83	GLU
16	P	2	VAL

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Mol	Chain	Res	Type
16	P	21	VAL
16	P	45	THR
16	P	60	LEU
16	P	62	VAL
17	Q	9	VAL
17	Q	36	ILE
17	Q	49	GLU
17	Q	63	ARG
17	Q	86	GLU
17	Q	91	ARG
18	R	26	LEU
18	R	37	VAL
18	R	41	LYS
18	R	76	LEU
18	R	84	LYS
19	S	5	LEU
19	S	27	GLU
19	S	37	ARG
19	S	41	VAL
19	S	65	ASN
19	S	77	THR
20	T	24	LEU
20	T	36	LEU
20	T	43	LEU
20	T	45	GLN
20	T	56	MET
20	T	80	ARG
20	T	90	GLN
21	U	10	ARG
21	U	12	LYS
21	U	24	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	78	GLN
2	B	95	GLN
3	C	6	HIS
3	C	28	GLN
3	C	98	ASN
3	C	102	ASN
3	C	104	GLN

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Mol	Chain	Res	Type
3	C	118	GLN
3	C	136	GLN
4	D	77	ASN
4	D	123	HIS
4	D	125	HIS
4	D	161	ASN
5	E	38	GLN
5	E	73	ASN
5	E	141	GLN
6	F	13	ASN
6	F	100	ASN
7	G	28	ASN
7	G	51	GLN
7	G	97	GLN
7	G	109	ASN
8	H	78	GLN
9	I	23	ASN
9	I	58	HIS
9	I	89	ASN
9	I	124	GLN
10	J	13	HIS
10	J	33	GLN
12	L	78	GLN
12	L	99	HIS
13	M	77	ASN
13	M	92	HIS
15	O	28	GLN
17	Q	16	GLN
19	S	23	ASN
19	S	47	HIS
19	S	65	ASN
20	T	9	ASN
20	T	75	ASN
20	T	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1501/1521 (98%)	306 (20%)	23 (1%)
22	V	12/24 (50%)	1 (8%)	0
23	W	68/76 (89%)	27 (39%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	Y	69/76 (90%)	28 (40%)	3 (4%)
24	X	75/77 (97%)	16 (21%)	1 (1%)
All	All	1725/1774 (97%)	378 (21%)	28 (1%)

All (378) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	66	G
1	A	73	G
1	A	78	G
1	A	79	G
1	A	80	G
1	A	88	A
1	A	89	C
1	A	91	C
1	A	92	C
1	A	96	U
1	A	101	A
1	A	111	G
1	A	116	A
1	A	121	C
1	A	131	C
1	A	138	G
1	A	142	G
1	A	144	G
1	A	155	C
1	A	156	G
1	A	163	C
1	A	166	G
1	A	172	A
1	A	174	C
1	A	179	A
1	A	180	U

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Mol	Chain	Res	Type
1	A	182	U
1	A	186	C
1	A	189	G
1	A	189(D)	C
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	226	G
1	A	247	G
1	A	251	G
1	A	258	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	332	G
1	A	344	A
1	A	345	C
1	A	352	C
1	A	353	A
1	A	354	G
1	A	355	C
1	A	367	U
1	A	372	C
1	A	373	A
1	A	381	C
1	A	384	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	414	A
1	A	424	G
1	A	426	G
1	A	429	U
1	A	430	A
1	A	439	A

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Mol	Chain	Res	Type
1	A	441	A
1	A	442	C
1	A	443	C
1	A	452	A
1	A	461	A
1	A	470	C
1	A	471	G
1	A	477	A
1	A	484	G
1	A	485	G
1	A	496	A
1	A	498	U
1	A	505	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	521	G
1	A	524	G
1	A	528	C
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	561	U
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	590	C
1	A	592	G
1	A	596	C
1	A	599	C
1	A	619	U
1	A	627	G
1	A	630	G
1	A	631	G
1	A	637	G
1	A	639	G
1	A	650	G
1	A	653	A

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Mol	Chain	Res	Type
1	A	660	G
1	A	665	A
1	A	673	G
1	A	687	A
1	A	688	G
1	A	695	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	749	C
1	A	752	G
1	A	755	G
1	A	759	A
1	A	773	G
1	A	774	G
1	A	777	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	816	A
1	A	817	C
1	A	821	G
1	A	828	A
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	859	A
1	A	873	A
1	A	874	G
1	A	902	G
1	A	913	A
1	A	914	A
1	A	926	G
1	A	927	G
1	A	931	C
1	A	932	C
1	A	934	C
1	A	936	C
1	A	960	U
1	A	961	U

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Mol	Chain	Res	Type
1	A	968	A
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	989	C
1	A	992	U
1	A	993	G
1	A	996	A
1	A	1000	U
1	A	1001(A)	G
1	A	1002	G
1	A	1003	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1008	C
1	A	1011	G
1	A	1021	G
1	A	1022	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1030	C
1	A	1030(A)	G
1	A	1032	G
1	A	1033	G
1	A	1035	A
1	A	1037	C
1	A	1039	C
1	A	1046	A
1	A	1052	U
1	A	1054	C
1	A	1055	A
1	A	1065	U
1	A	1066	C

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Mol	Chain	Res	Type
1	A	1067	A
1	A	1068	G
1	A	1077	G
1	A	1081	G
1	A	1085	U
1	A	1088	G
1	A	1089	G
1	A	1094	G
1	A	1095	U
1	A	1097	C
1	A	1101	A
1	A	1104	G
1	A	1108	G
1	A	1110	A
1	A	1111	A
1	A	1117	G
1	A	1118	C
1	A	1129	C
1	A	1130	A
1	A	1132	C
1	A	1134	G
1	A	1135	U
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1146	A
1	A	1147	C
1	A	1151	A
1	A	1152	A
1	A	1154	G
1	A	1157	A
1	A	1158	C
1	A	1159	U
1	A	1161	C
1	A	1165	C
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1190	G

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Mol	Chain	Res	Type
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1222	G
1	A	1224	G
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1240	U
1	A	1250	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1269	A
1	A	1270	C
1	A	1273	G
1	A	1276	G
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1287	A
1	A	1300	G
1	A	1305	G
1	A	1317	C
1	A	1320	C
1	A	1338	G
1	A	1340	A
1	A	1347	G
1	A	1353	G
1	A	1357	A
1	A	1358	U
1	A	1363	C
1	A	1370	G
1	A	1379	G
1	A	1394	A
1	A	1397	C

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Mol	Chain	Res	Type
1	A	1419	G
1	A	1442	G
1	A	1442(A)	G
1	A	1446	U
1	A	1447	A
1	A	1456	G
1	A	1475	G
1	A	1492	A
1	A	1493	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U
22	V	13	A
23	W	3	C
23	W	4	C
23	W	6	G
23	W	8	4SU
23	W	9	A
23	W	12	U
23	W	14	A
23	W	19	G
23	W	22	G
23	W	25	C
23	W	26	A
23	W	27	G
23	W	29	G
23	W	34	G
23	W	46	7MG
23	W	48	C
23	W	49	C
23	W	50	U
23	W	61	C
23	W	62	C
23	W	63	G
23	W	64	A

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Mol	Chain	Res	Type
23	W	66	U
23	W	68	C
23	W	70	G
23	W	73	A
23	W	74	C
24	X	9	G
24	X	16	C
24	X	18	G
24	X	19	G
24	X	20	U
24	X	21	A
24	X	31	G
24	X	46	G
24	X	47	U
24	X	48	C
24	X	50	U
24	X	54	5MU
24	X	56	C
24	X	64	G
24	X	68	C
24	X	76	A
23	Y	3	C
23	Y	11	C
23	Y	13	C
23	Y	14	A
23	Y	15	G
23	Y	19	G
23	Y	23	A
23	Y	24	G
23	Y	25	C
23	Y	34	G
23	Y	44	G
23	Y	45	U
23	Y	47	U
23	Y	48	C
23	Y	49	C
23	Y	52	G
23	Y	54	5MU
23	Y	55	PSU
23	Y	56	C
23	Y	57	G
23	Y	58	A

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Mol	Chain	Res	Type
23	Y	59	U
23	Y	61	C
23	Y	62	C
23	Y	65	G
23	Y	68	C
23	Y	70	G
23	Y	73	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	65	U
1	A	115	G
1	A	250	A
1	A	266	G
1	A	429	U
1	A	509	A
1	A	560	U
1	A	687	A
1	A	748	C
1	A	839	U
1	A	913	A
1	A	1027	C
1	A	1064	G
1	A	1065	U
1	A	1067	A
1	A	1128	C
1	A	1181	G
1	A	1183	A
1	A	1190	G
1	A	1201	A
1	A	1212	U
1	A	1442	G
1	A	1492	A
23	W	13	C
24	X	16	C
23	Y	14	A
23	Y	46	7MG
23	Y	58	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
23	PSU	W	32	23	19,21,22	1.78	4 (21%)	23,30,33	1.00	2 (8%)
23	MIA	W	37	23	24,27,32	1.96	6 (25%)	35,39,47	2.01	7 (20%)
23	PSU	W	39	23	19,21,22	1.85	5 (26%)	23,30,33	0.96	1 (4%)
23	7MG	W	46	23	24,26,27	2.00	6 (25%)	34,39,42	2.28	8 (23%)
23	5MU	W	54	23	20,22,23	1.66	4 (20%)	25,32,35	1.78	4 (16%)
23	PSU	W	55	23	19,21,22	1.77	4 (21%)	23,30,33	1.35	2 (8%)
23	4SU	W	8	23	19,21,22	1.80	4 (21%)	23,30,33	2.77	3 (13%)
24	5MC	X	32	24	20,22,23	1.80	4 (20%)	26,32,35	1.48	4 (15%)
24	5MU	X	54	24	20,22,23	1.70	4 (20%)	25,32,35	2.07	4 (16%)
24	PSU	X	55	24	19,21,22	1.78	4 (21%)	23,30,33	0.98	1 (4%)
24	4SU	X	8	24	19,21,22	1.72	4 (21%)	23,30,33	29.03	2 (8%)
23	PSU	Y	32	23	19,21,22	1.78	4 (21%)	23,30,33	0.95	2 (8%)
23	MIA	Y	37	23	20,24,32	1.71	5 (25%)	27,35,47	1.95	5 (18%)
23	PSU	Y	39	23	19,21,22	1.90	4 (21%)	23,30,33	1.51	2 (8%)
23	7MG	Y	46	23	24,26,27	2.05	8 (33%)	34,39,42	2.73	12 (35%)
23	5MU	Y	54	23	20,22,23	1.85	4 (20%)	25,32,35	2.01	5 (20%)
23	PSU	Y	55	23	19,21,22	1.87	6 (31%)	23,30,33	1.03	3 (13%)
23	4SU	Y	8	23	19,21,22	1.85	4 (21%)	23,30,33	7.20	4 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	W	32	23	-	0/8/25/26	0/2/2/2
23	MIA	W	37	23	-	0/12/29/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	W	39	23	-	0/8/25/26	0/2/2/2
23	7MG	W	46	23	-	0/8/37/38	0/3/3/3
23	5MU	W	54	23	-	0/6/25/26	0/2/2/2
23	PSU	W	55	23	-	0/8/25/26	0/2/2/2
23	4SU	W	8	23	-	0/6/25/26	0/2/2/2
24	5MC	X	32	24	-	0/6/25/26	0/2/2/2
24	5MU	X	54	24	-	0/6/25/26	0/2/2/2
24	PSU	X	55	24	-	0/8/25/26	0/2/2/2
24	4SU	X	8	24	-	0/6/25/26	0/2/2/2
23	PSU	Y	32	23	-	0/8/25/26	0/2/2/2
23	MIA	Y	37	23	-	0/8/25/34	0/3/3/3
23	PSU	Y	39	23	-	0/8/25/26	0/2/2/2
23	7MG	Y	46	23	-	0/8/37/38	0/3/3/3
23	5MU	Y	54	23	-	1/6/25/26	0/2/2/2
23	PSU	Y	55	23	-	0/8/25/26	0/2/2/2
23	4SU	Y	8	23	-	0/6/25/26	0/2/2/2

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	37	MIA	C2-S10	-6.01	1.70	1.75
23	W	46	7MG	C6-C5	5.83	1.48	1.41
24	X	32	5MC	C5-C4	4.88	1.49	1.41
23	Y	8	4SU	P-OP1	4.68	1.52	1.46
23	Y	46	7MG	C6-C5	4.66	1.47	1.41
23	Y	54	5MU	P-OP1	4.53	1.51	1.46
23	W	46	7MG	P-OP1	4.50	1.51	1.46
23	Y	55	PSU	P-OP1	4.48	1.51	1.46
24	X	8	4SU	P-OP1	4.48	1.51	1.46
23	W	55	PSU	P-OP1	4.48	1.51	1.46
23	Y	46	7MG	P-OP1	4.48	1.51	1.46
23	W	8	4SU	P-OP1	4.42	1.51	1.46
23	W	39	PSU	P-OP1	4.38	1.51	1.46
23	Y	37	MIA	P-OP1	4.34	1.51	1.46
23	Y	39	PSU	P-OP1	4.32	1.51	1.46
23	Y	39	PSU	C5-C1'	-4.27	1.48	1.52
23	W	54	5MU	P-OP1	4.26	1.51	1.46
23	Y	32	PSU	P-OP1	4.20	1.51	1.46
23	Y	54	5MU	C2-N1	4.18	1.42	1.38
24	X	55	PSU	P-OP1	4.11	1.51	1.46
24	X	54	5MU	P-OP1	4.09	1.51	1.46
24	X	32	5MC	P-OP1	4.08	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	37	MIA	P-OP1	4.04	1.51	1.46
23	W	32	PSU	P-OP1	4.00	1.51	1.46
23	Y	8	4SU	C2-N1	3.94	1.42	1.38
23	Y	8	4SU	C4-S4	-3.82	1.60	1.67
23	W	32	PSU	C4-C5	3.81	1.49	1.40
23	Y	55	PSU	C5-C1'	-3.74	1.48	1.52
23	W	8	4SU	C2-N1	3.72	1.42	1.38
24	X	55	PSU	C4-C5	3.69	1.49	1.40
23	W	8	4SU	C4-S4	-3.62	1.60	1.67
24	X	54	5MU	C4-C5	3.59	1.49	1.40
24	X	32	5MC	C2-N1	3.58	1.42	1.38
23	Y	32	PSU	C5-C1'	-3.58	1.49	1.52
23	Y	46	7MG	C2-N3	3.54	1.37	1.33
23	W	39	PSU	C4-C5	3.52	1.49	1.40
24	X	8	4SU	O2-C2	3.50	1.26	1.21
23	W	39	PSU	C5-C1'	-3.50	1.49	1.52
24	X	8	4SU	C4-S4	-3.50	1.60	1.67
23	Y	55	PSU	C4-C5	3.47	1.48	1.40
23	Y	54	5MU	C4-C5	3.46	1.48	1.40
24	X	54	5MU	C2-N1	3.43	1.42	1.38
23	Y	32	PSU	C4-C5	3.41	1.48	1.40
23	W	54	5MU	C4-C5	3.39	1.48	1.40
23	W	55	PSU	C4-C5	3.39	1.48	1.40
23	Y	37	MIA	C5-C4	3.32	1.48	1.40
23	Y	37	MIA	C6-N6	3.31	1.35	1.28
23	W	32	PSU	C5-C1'	-3.30	1.49	1.52
23	Y	39	PSU	C4-C5	3.27	1.48	1.40
23	W	54	5MU	C2-N1	3.18	1.41	1.38
23	W	37	MIA	C5-C4	3.16	1.47	1.40
23	Y	54	5MU	O2-C2	3.15	1.25	1.21
23	W	8	4SU	O2-C2	3.15	1.25	1.21
23	Y	46	7MG	C5-N7	-3.14	1.33	1.39
23	W	39	PSU	O2-C2	3.12	1.25	1.21
23	W	54	5MU	O2-C2	3.08	1.25	1.21
23	W	55	PSU	C5-C1'	-3.08	1.49	1.52
24	X	55	PSU	C5-C1'	-3.08	1.49	1.52
23	Y	32	PSU	O2-C2	3.07	1.25	1.21
23	Y	39	PSU	O2-C2	3.07	1.25	1.21
24	X	55	PSU	O2-C2	3.02	1.25	1.21
23	W	32	PSU	O2-C2	2.98	1.25	1.21
23	W	55	PSU	O2-C2	2.94	1.25	1.21
23	Y	46	7MG	C5-C4	2.73	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	46	7MG	C2-N2	2.72	1.36	1.32
24	X	32	5MC	O2-C2	2.69	1.25	1.21
23	W	46	7MG	C5-N7	-2.66	1.34	1.39
24	X	54	5MU	O2-C2	2.59	1.25	1.21
23	W	37	MIA	C4-N9	-2.56	1.34	1.37
23	Y	8	4SU	O2-C2	2.55	1.25	1.21
23	W	46	7MG	C5-C4	2.50	1.47	1.39
23	W	46	7MG	C2-N3	2.45	1.36	1.33
23	W	37	MIA	C6-C5	2.39	1.48	1.44
24	X	8	4SU	C2-N1	2.35	1.41	1.38
23	W	46	7MG	C2-N2	2.33	1.35	1.32
23	Y	55	PSU	C4-N3	-2.30	1.33	1.36
23	Y	37	MIA	C4-N9	-2.29	1.34	1.37
23	W	37	MIA	C6-N1	2.12	1.36	1.33
23	Y	37	MIA	C6-C5	2.11	1.48	1.44
23	Y	55	PSU	O2-C2	2.07	1.24	1.21
23	Y	46	7MG	CM7-N7	2.06	1.49	1.46
23	Y	46	7MG	C8-N9	2.05	1.47	1.46
23	Y	55	PSU	O4'-C1'	-2.02	1.41	1.44
23	W	39	PSU	C4-N3	-2.01	1.33	1.36

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	8	4SU	C4-N3-C2	138.99	127.55	121.60
23	Y	8	4SU	C4-N3-C2	-33.30	120.18	121.60
23	W	8	4SU	C4-N3-C2	10.15	122.04	121.60
23	Y	46	7MG	N3-C4-N9	8.80	140.70	126.80
24	X	8	4SU	C2-N1-C1'	7.91	123.17	118.21
23	W	46	7MG	N3-C4-N9	7.14	138.09	126.80
24	X	54	5MU	N3-C2-N1	6.91	121.74	115.97
23	W	8	4SU	C2-N1-C1'	6.67	122.39	118.21
23	Y	46	7MG	C6-N1-C2	6.45	123.84	120.20
23	W	37	MIA	C5-C4-N3	-6.40	118.70	126.07
23	Y	8	4SU	N3-C2-N1	6.33	121.25	115.97
23	Y	54	5MU	N3-C2-N1	6.25	121.19	115.97
23	Y	37	MIA	C5-C4-N3	-6.11	119.03	126.07
23	Y	37	MIA	N3-C4-N9	5.92	135.59	126.91
23	W	46	7MG	N7-C8-N9	-5.77	95.46	103.13
23	Y	39	PSU	C5-C1'-C2'	-5.76	105.05	115.73
23	Y	46	7MG	C5-C4-N3	-5.71	116.60	126.61
24	X	54	5MU	C6-N1-C2	-5.70	120.79	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	54	5MU	C6-N1-C2	-5.46	120.86	122.41
23	W	37	MIA	N3-C4-N9	5.35	134.76	126.91
23	W	54	5MU	C6-N1-C2	-5.33	120.89	122.41
23	W	54	5MU	N3-C2-N1	5.33	120.42	115.97
23	Y	8	4SU	C2-N1-C1'	5.25	121.50	118.21
24	X	32	5MC	C2-N3-C4	5.10	120.38	115.50
23	W	46	7MG	C5-C4-N3	-5.05	117.77	126.61
23	Y	46	7MG	N7-C8-N9	-4.78	96.79	103.13
23	W	55	PSU	C5-C1'-C2'	-4.77	106.89	115.73
23	W	37	MIA	C2-N3-C4	4.48	121.53	115.22
23	W	8	4SU	N3-C2-N1	4.46	119.69	115.97
23	W	46	7MG	C8-N7-C5	3.79	116.40	108.83
23	Y	46	7MG	C8-N9-C1'	-3.64	111.02	121.06
23	W	46	7MG	C6-N1-C2	3.56	122.21	120.20
23	W	37	MIA	C4-C5-N7	-3.29	106.23	109.41
23	Y	46	7MG	C8-N7-C5	3.27	115.35	108.83
23	Y	46	7MG	C6-C5-C4	3.22	120.40	116.01
24	X	54	5MU	C5-C6-N1	-3.16	119.18	122.02
23	W	37	MIA	C2-N1-C6	3.02	122.26	113.31
23	Y	54	5MU	C5-C6-N1	-2.96	119.36	122.02
23	Y	37	MIA	C5-C6-N1	-2.94	117.54	120.10
23	Y	46	7MG	N2-C2-N1	-2.92	114.69	117.82
23	W	54	5MU	C2-N1-C1'	2.92	120.04	118.21
23	W	37	MIA	C5-C6-N1	-2.85	117.42	120.46
23	W	39	PSU	C5-C1'-C2'	-2.62	110.86	115.73
23	Y	54	5MU	C2-N1-C1'	2.59	119.83	118.21
23	Y	37	MIA	C8-N9-C4	2.59	109.06	106.96
24	X	32	5MC	C5-C6-N1	-2.50	119.77	122.02
24	X	32	5MC	C6-N1-C2	2.49	120.64	118.86
23	W	37	MIA	N3-C2-N1	-2.48	122.39	126.87
24	X	54	5MU	C4-N3-C2	-2.47	120.33	125.39
24	X	32	5MC	N4-C4-N3	2.45	120.49	116.99
24	X	55	PSU	C4-N3-C2	-2.40	120.49	125.36
23	Y	54	5MU	C4-N3-C2	-2.40	120.47	125.39
23	W	32	PSU	C5-C1'-C2'	-2.39	111.30	115.73
23	W	46	7MG	C6-C5-C4	2.37	119.23	116.01
23	Y	8	4SU	C5-C4-N3	2.36	120.13	116.04
23	Y	55	PSU	C5-C1'-C2'	-2.34	111.39	115.73
23	Y	32	PSU	C5-C1'-C2'	-2.33	111.41	115.73
23	Y	46	7MG	C5-C4-N9	-2.28	102.66	106.08
23	W	46	7MG	C8-N9-C4	2.27	117.84	110.66
23	Y	37	MIA	C4-C5-N7	-2.26	107.23	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	46	7MG	CM7-N7-C5	2.25	131.65	123.46
23	W	55	PSU	C4-N3-C2	-2.25	120.80	125.36
23	W	32	PSU	C4-N3-C2	-2.18	120.94	125.36
23	Y	32	PSU	C4-N3-C2	-2.17	120.95	125.36
23	Y	55	PSU	O4'-C1'-C2'	2.12	108.05	104.43
23	Y	55	PSU	C4-N3-C2	-2.11	121.09	125.36
23	Y	39	PSU	C4-N3-C2	-2.10	121.10	125.36
23	Y	46	7MG	C4-N9-C1'	2.07	131.72	126.62
23	Y	46	7MG	C8-N9-C4	2.05	117.16	110.66
23	W	54	5MU	C5-C6-N1	-2.03	120.20	122.02
23	W	46	7MG	CM7-N7-C5	2.01	130.77	123.46

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Y	54	5MU	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 232 ligands modelled in this entry, 230 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
26	UAM	A	3202	-	31,31,31	1.44	2 (6%)	44,44,44	1.38	7 (15%)
27	SF4	D	501	4	12,12,12	21.81	12 (100%)	0,24,24	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	UAM	A	3202	-	-	0/28/40/40	0/2/2/2
27	SF4	D	501	4	-	0/0/48/48	0/6/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	501	SF4	S4-FE2	-22.39	2.18	2.33
27	D	501	SF4	S3-FE2	-22.18	2.18	2.33
27	D	501	SF4	S4-FE1	-22.15	2.18	2.33
27	D	501	SF4	S3-FE1	-22.09	2.18	2.33
27	D	501	SF4	S1-FE3	-21.99	2.18	2.33
27	D	501	SF4	S2-FE4	-21.97	2.18	2.33
27	D	501	SF4	S2-FE3	-21.71	2.18	2.33
27	D	501	SF4	S4-FE3	-21.69	2.18	2.33
27	D	501	SF4	S2-FE1	-21.59	2.18	2.33
27	D	501	SF4	S1-FE4	-21.40	2.18	2.33
27	D	501	SF4	S3-FE4	-21.30	2.18	2.33
27	D	501	SF4	S1-FE2	-21.28	2.18	2.33
26	A	3202	UAM	CAO-CAW	-6.71	1.39	1.51
26	A	3202	UAM	CAX-CAU	-2.82	1.38	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	3202	UAM	CAO-CBD-CBC	-4.53	109.27	116.45
26	A	3202	UAM	CBD-OAR-CAU	-3.24	113.71	118.73
26	A	3202	UAM	OAR-CAU-OAG	2.80	121.32	117.68
26	A	3202	UAM	CAP-CBC-CBD	-2.65	108.58	112.59
26	A	3202	UAM	OAH-CAV-CAX	-2.32	116.59	121.11
26	A	3202	UAM	CAZ-CAN-CAS	-2.28	109.63	112.79
26	A	3202	UAM	CAY-CAP-CBC	-2.28	109.99	115.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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