



Full wwPDB X-ray Structure Validation Report

Oct 10, 2014 – 01:46 PM EDT

PDB ID : 4RB9
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with pactamycin (soaked), 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 : 2.55 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>

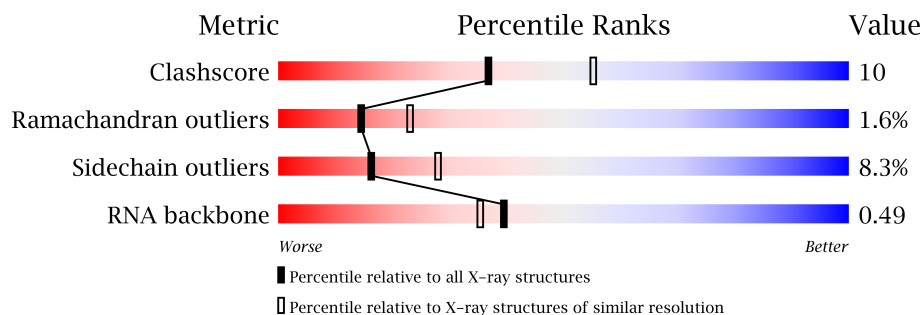
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.55 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	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RNA backbone	1838	1058 (3.10-1.98)







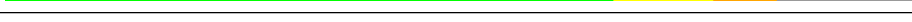

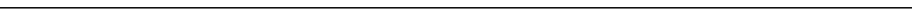


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The 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 56420 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	1498	Total	C	N	O	P	0	0	0
			32205	14333	5970	10404	1498			

- 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
			1846	1179	331	331	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
			1552	976	302	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
			1659	1040	326	286	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
			1129	714	213	198	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			806	511	143	149	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
			1231	766	243	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
			983	623	193	167			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	97	Total	C	N	O	0	0	0
			709	440	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
			829	516	155	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	123	Total	C	N	O	S	0	0	0
			958	592	198	166	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
			681	433	134	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
			652	417	120	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
			728	446	156	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	74	Total	C	N	O	P	S	0	0	0
			1588	713	285	515	73	2			
23	Y	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	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).

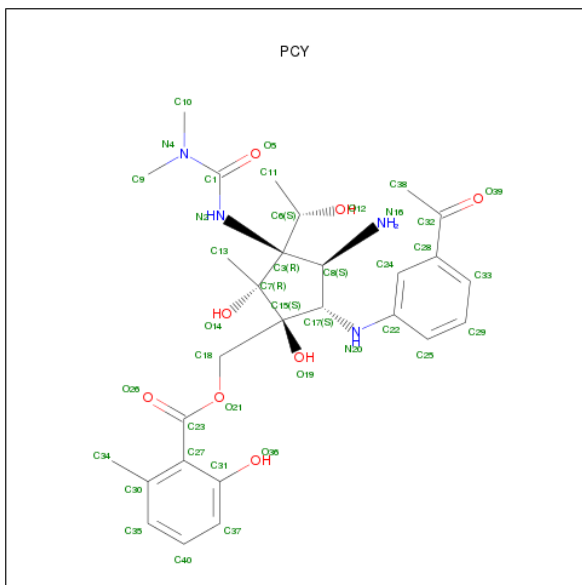
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	D	1	Total	Mg	0	0
			1	1		
25	K	2	Total	Mg	0	0
			2	2		
25	E	1	Total	Mg	0	0
			1	1		
25	V	1	Total	Mg	0	0
			1	1		
25	W	7	Total	Mg	0	0
			7	7		
25	A	230	Total	Mg	0	0
			230	230		
25	N	1	Total	Mg	0	0
			1	1		
25	X	12	Total	Mg	0	0
			12	12		

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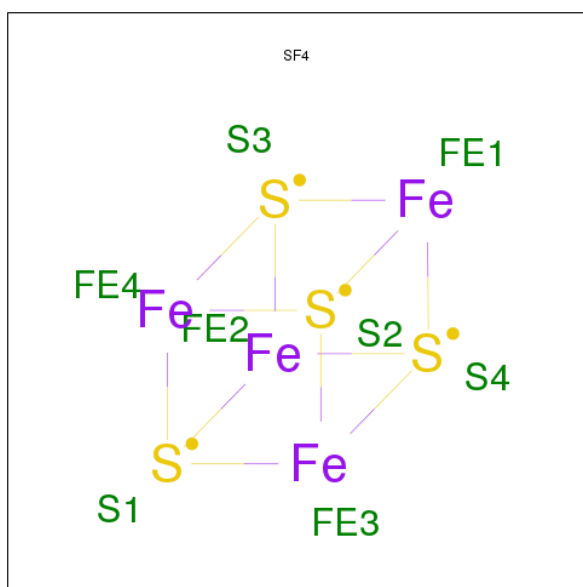
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	Y	3	Total Mg 3 3	0	0
25	F	1	Total Mg 1 1	0	0
25	M	1	Total Mg 1 1	0	0

- Molecule 26 is PACTAMYCIN (three-letter code: PCY) (formula: $C_{28}H_{38}N_4O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			40	28	4	8		

- 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	226	Total	O	0	0
			226	226		
30	E	3	Total	O	0	0
			3	3		
30	J	1	Total	O	0	0
			1	1		
30	L	4	Total	O	0	0
			4	4		

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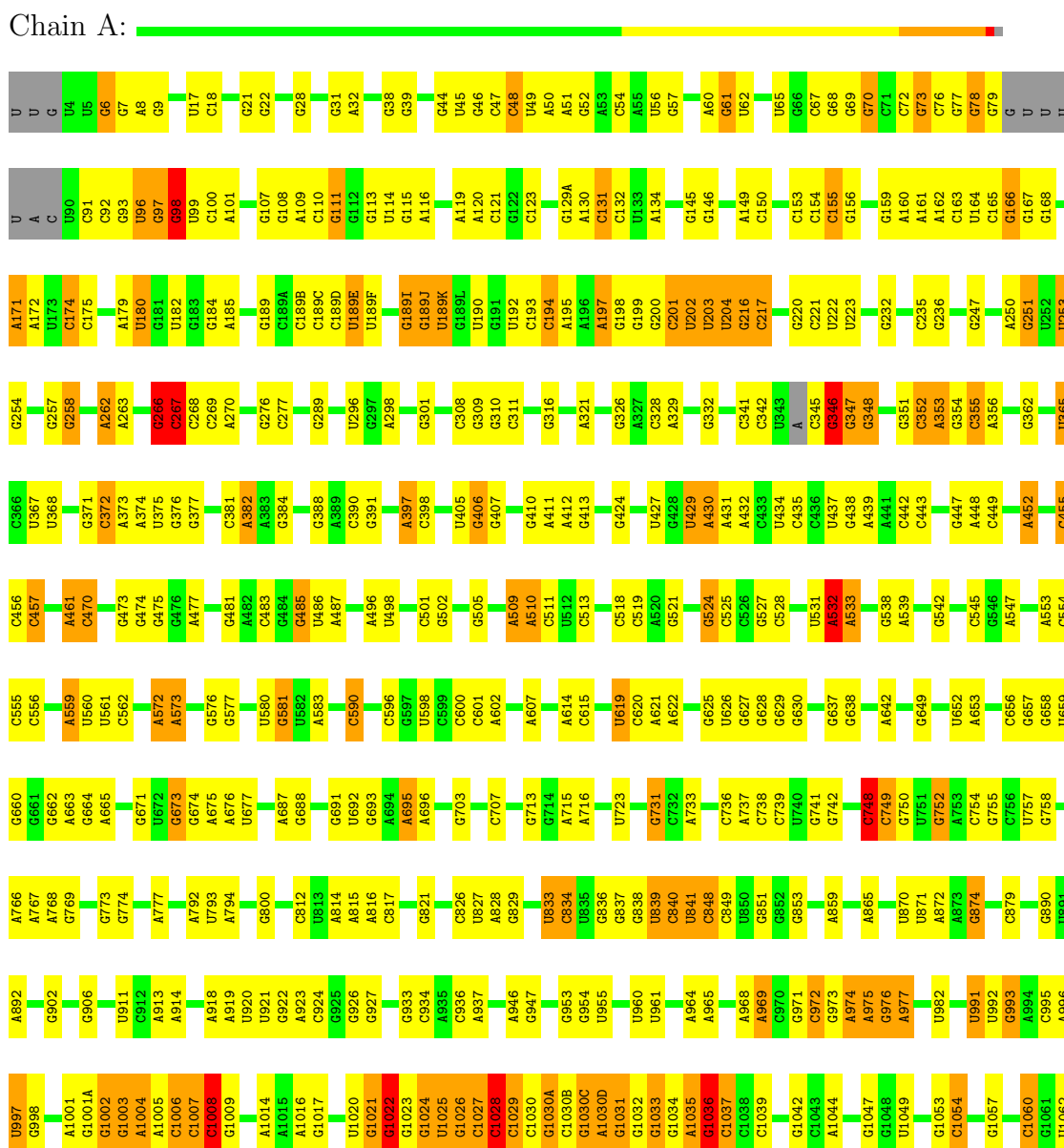
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	M	1	Total	O	0	0
			1	1		
30	V	4	Total	O	0	0
			4	4		
30	W	6	Total	O	0	0
			6	6		
30	X	8	Total	O	0	0
			8	8		
30	Y	3	Total	O	0	0
			3	3		

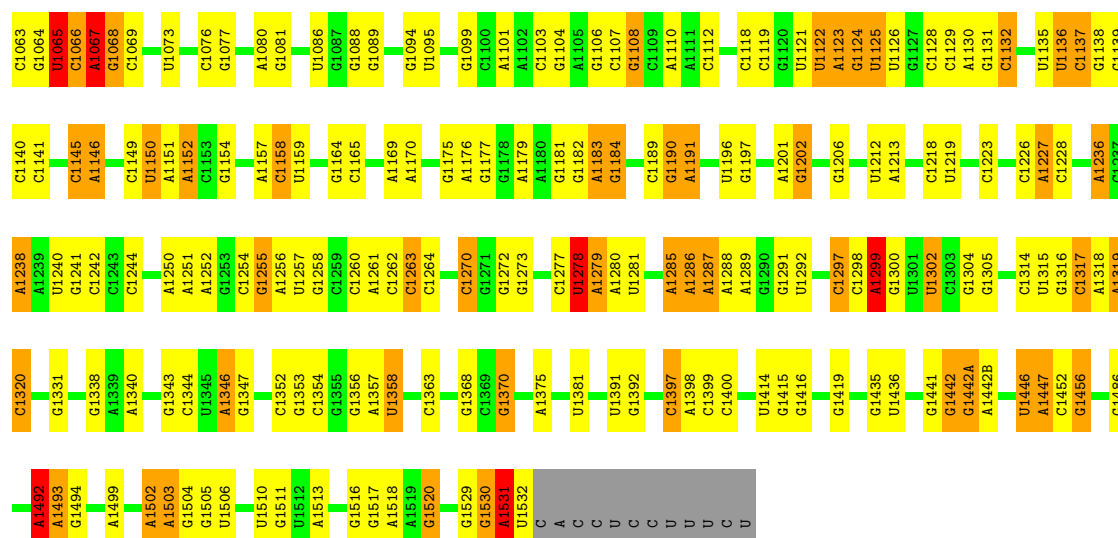
3 Residue-property plots

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.

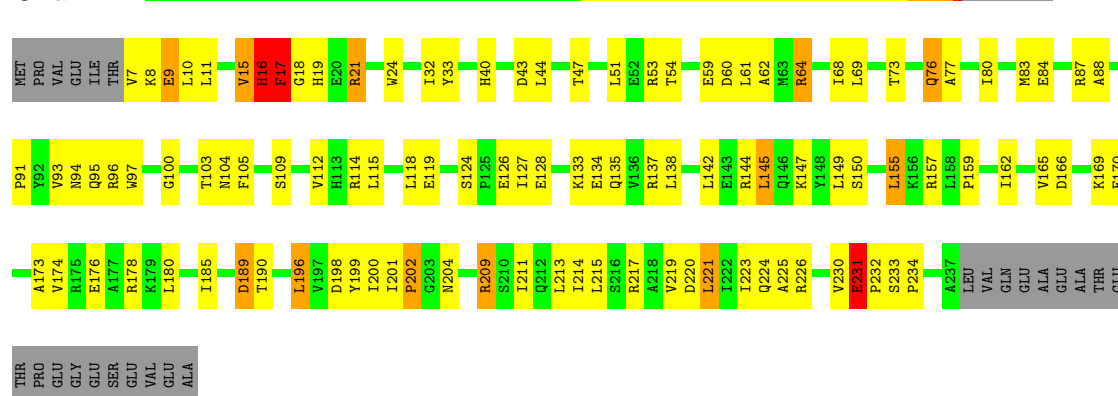
• Molecule 1: 16S Ribosomal RNA





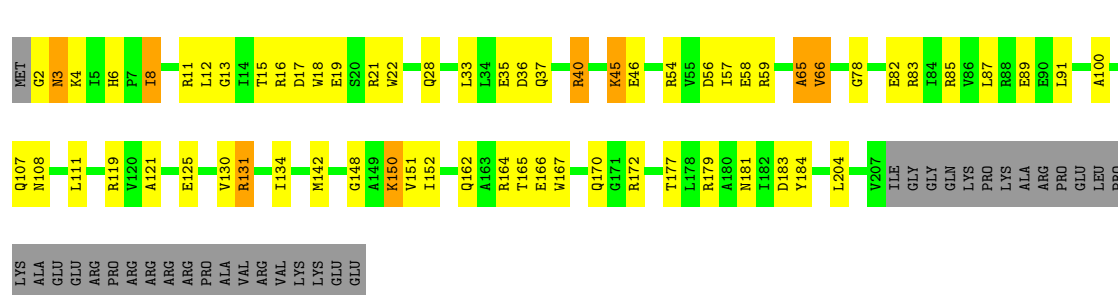
- Molecule 2: 30S Ribosomal Protein S2

Chain B:



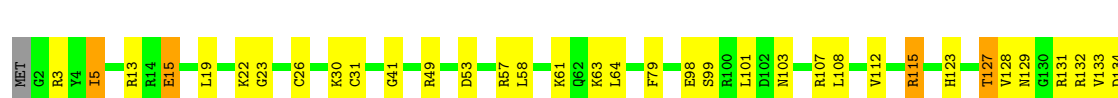
- Molecule 3: 30S Ribosomal Protein S3

Chain C:



- Molecule 4: 30S Ribosomal Protein S4

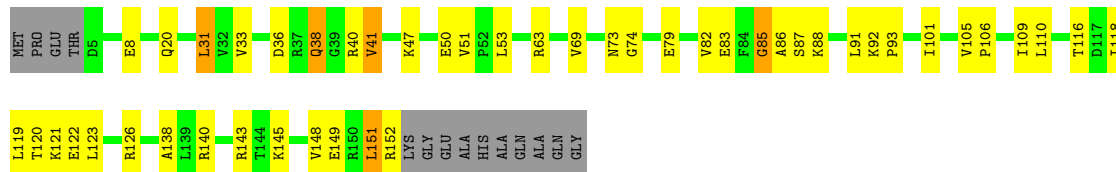
Chain D:





• Molecule 5: 30S Ribosomal Protein S5

Chain E:



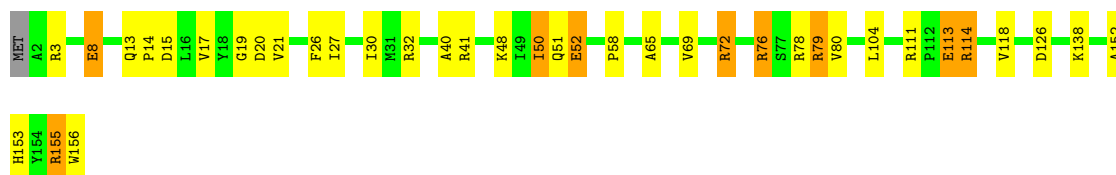
• Molecule 6: 30S Ribosomal Protein S6

Chain F:



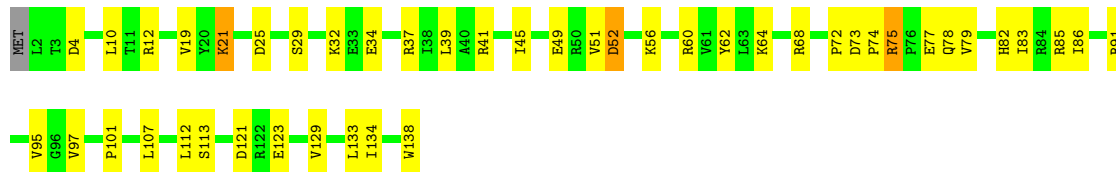
• Molecule 7: 30S Ribosomal Protein S7

Chain G:



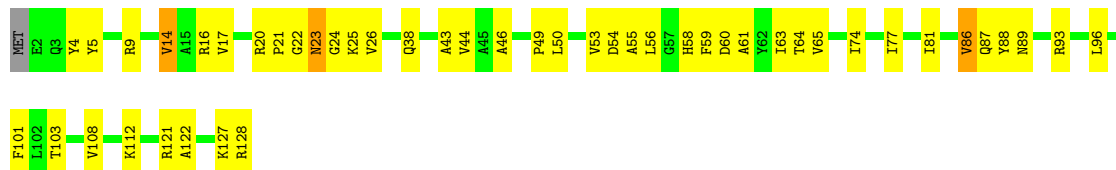
• Molecule 8: 30S Ribosomal Protein S8

Chain H:



• Molecule 9: 30S Ribosomal Protein S9

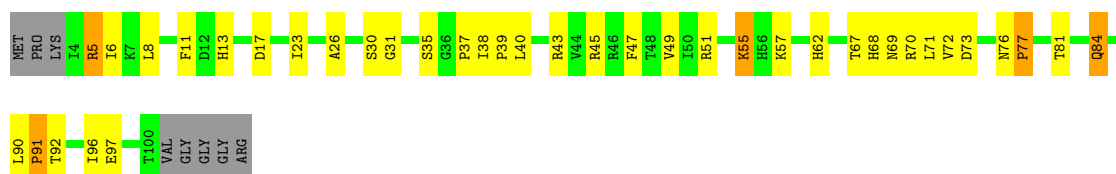
Chain I:



• Molecule 10: 30S Ribosomal Protein S10

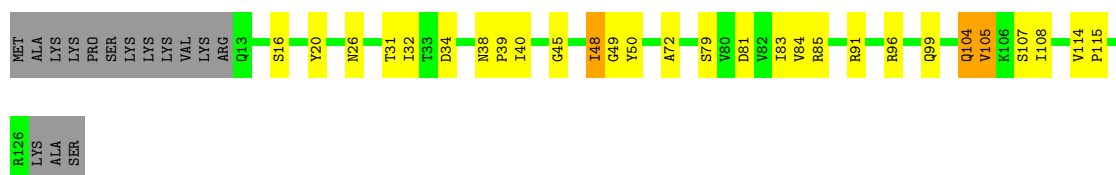
Chain J:





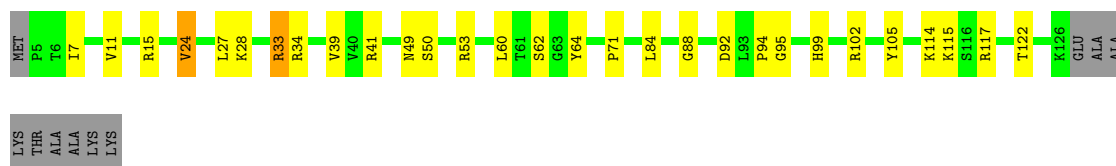
• Molecule 11: 30S Ribosomal Protein S11

Chain K:



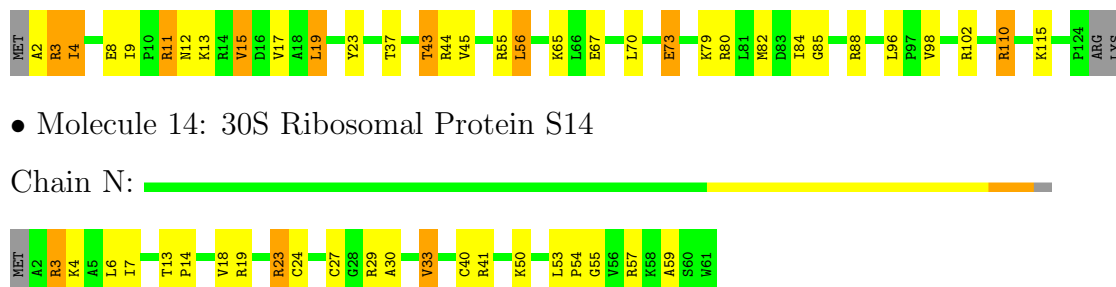
• Molecule 12: 30S Ribosomal Protein S12

Chain L:



• Molecule 13: 30S Ribosomal Protein S13

Chain M:



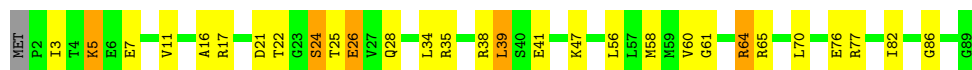
• Molecule 14: 30S Ribosomal Protein S14

Chain N:



• Molecule 15: 30S Ribosomal Protein S15

Chain O:



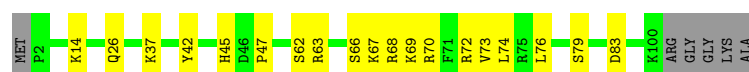
• Molecule 16: 30S Ribosomal Protein S16

Chain P:



• Molecule 17: 30S Ribosomal Protein S17

Chain Q: 



- Molecule 18: 30S Ribosomal Protein S18

Chain R: 



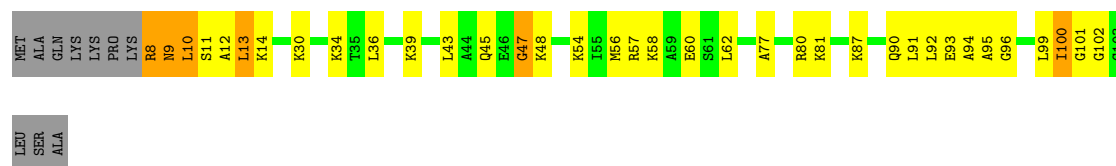
- Molecule 19: 30S Ribosomal Protein S19

Chain S: 



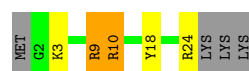
- Molecule 20: 30S Ribosomal Protein S20

Chain T: 



- Molecule 21: 30S Ribosomal Protein THX

Chain U: 



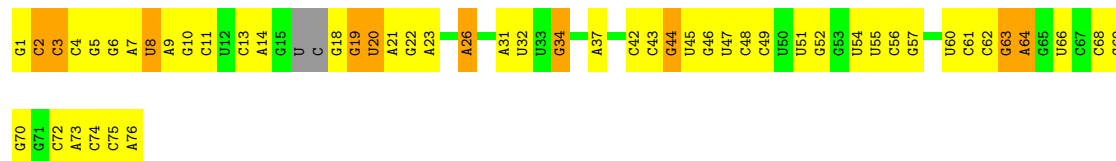
- Molecule 22: mRNA

Chain V: 



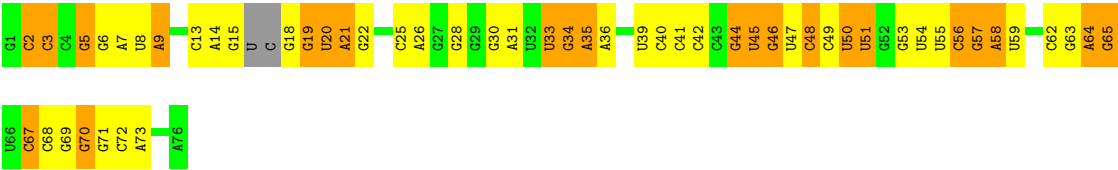
- Molecule 23: A/P-site tRNA

Chain W: 



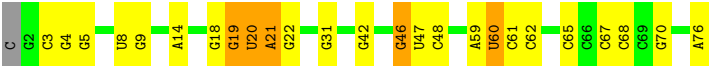
- Molecule 23: A/P-site tRNA

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	209.35Å 449.01Å 621.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.52 – 2.55	Depositor
% Data completeness (in resolution range)	99.0 (145.52-2.55)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.225 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	56420	wwPDB-VP
Average B, all atoms (Å ²)	69.0	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, PCY, MIA, SF4, MG, 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	0.43	0/36049	0.93	45/56261 (0.1%)
2	B	0.31	0/1881	0.62	1/2542 (0.0%)
3	C	0.30	0/1576	0.52	0/2130
4	D	0.32	0/1689	0.53	0/2267
5	E	0.31	0/1145	0.54	0/1543
6	F	0.32	0/819	0.53	0/1111
7	G	0.30	0/1250	0.49	0/1679
8	H	0.30	0/1108	0.51	0/1494
9	I	0.32	0/1002	0.56	0/1346
10	J	0.30	0/722	0.56	0/982
11	K	0.31	0/844	0.54	0/1145
12	L	0.33	0/946	0.53	0/1274
13	M	0.30	0/969	0.57	0/1302
14	N	0.34	0/501	0.50	0/664
15	O	0.30	0/739	0.56	0/985
16	P	0.32	0/697	0.53	0/939
17	Q	0.31	0/836	0.49	0/1117
18	R	0.32	0/560	0.55	0/746
19	S	0.30	0/667	0.54	0/900
20	T	0.29	0/730	0.57	0/965
21	U	0.33	0/203	0.50	0/266
22	V	0.48	0/310	1.00	0/480
23	W	0.48	0/1602	1.06	0/2493
23	Y	0.52	0/1602	1.16	4/2493 (0.2%)
24	X	0.55	2/1725 (0.1%)	1.16	12/2689 (0.4%)
All	All	0.41	2/60172 (0.0%)	0.86	62/89813 (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
2	B	0	1
7	G	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	X	14	A	N7-C5	-6.24	1.35	1.39
24	X	14	A	C8-N7	-6.01	1.27	1.31

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	14	A	C4-C5-C6	10.08	122.04	117.00
24	X	46	G	C6-N1-C2	-9.82	119.21	125.10
24	X	14	A	C5-N7-C8	9.60	108.70	103.90
23	Y	64	A	C5-C6-N6	8.55	130.54	123.70
24	X	14	A	C5-C6-N1	-8.12	113.64	117.70
23	Y	64	A	N1-C6-N6	-7.87	113.88	118.60
24	X	22	G	C5-N7-C8	-7.87	100.37	104.30
1	A	365	U	C5-C6-N1	-7.12	119.14	122.70
1	A	1397	C	O4'-C1'-N1	7.10	113.88	108.20
1	A	991	U	P-O3'-C3'	7.09	128.21	119.70
1	A	254	G	O5'-P-OP1	-7.05	99.36	105.70
1	A	1030(B)	C	C2-N1-C1'	6.98	126.47	118.80
24	X	46	G	C5-C6-N1	6.87	114.93	111.50
1	A	98	G	N3-C4-N9	6.68	130.01	126.00
1	A	1278	U	C5-C6-N1	6.64	126.02	122.70
1	A	1002	G	N3-C4-N9	6.53	129.92	126.00
1	A	98	G	C6-C5-N7	-6.51	126.49	130.40
1	A	1030(B)	C	O4'-C1'-N1	6.47	113.37	108.20
1	A	1397	C	C2-N1-C1'	6.42	125.86	118.80
1	A	98	G	N7-C8-N9	6.13	116.17	113.10
1	A	365	U	C2-N1-C1'	-6.12	110.35	117.70
1	A	1036	G	N1-C6-O6	-5.96	116.32	119.90
1	A	1002	G	N3-C4-C5	-5.92	125.64	128.60
23	Y	64	A	C6-N1-C2	5.84	122.11	118.60
1	A	98	G	N3-C4-C5	-5.81	125.69	128.60
1	A	267	C	O5'-P-OP1	-5.74	100.54	105.70
1	A	98	G	C4-N9-C1'	5.73	133.95	126.50
1	A	1502	A	N7-C8-N9	5.73	116.66	113.80
23	Y	50	U	C2-N3-C4	5.67	130.40	127.00
24	X	14	A	C8-N9-C1'	-5.66	117.52	127.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1067	A	P-O3'-C3'	5.64	126.47	119.70
1	A	266	G	P-O3'-C3'	5.64	126.47	119.70
1	A	1007	C	C2-N3-C4	5.59	122.70	119.90
1	A	346	G	C4-N9-C1'	5.57	133.74	126.50
1	A	1299	A	O5'-P-OP1	5.55	117.36	110.70
1	A	1190	G	OP2-P-O3'	5.54	117.39	105.20
1	A	754	C	C2-N1-C1'	5.51	124.86	118.80
24	X	22	G	N7-C8-N9	5.50	115.85	113.10
1	A	1008	C	C2-N3-C4	5.48	122.64	119.90
1	A	1007	C	N1-C2-O2	5.48	122.19	118.90
1	A	1022	G	N3-C2-N2	5.45	123.71	119.90
1	A	1397	C	C6-N1-C1'	-5.42	114.30	120.80
2	B	9	GLU	N-CA-C	5.41	125.60	111.00
24	X	14	A	C4-N9-C1'	5.40	136.02	126.30
1	A	1002	G	C4-N9-C1'	5.38	133.50	126.50
1	A	1285	A	P-O3'-C3'	5.37	126.14	119.70
24	X	22	G	C4-C5-C6	-5.33	115.60	118.80
1	A	346	G	O4'-C1'-N9	5.32	112.46	108.20
1	A	1036	G	C4-N9-C1'	5.32	133.42	126.50
1	A	532	A	P-O3'-C3'	5.27	126.03	119.70
1	A	1492	A	P-O3'-C3'	5.26	126.01	119.70
1	A	1028	C	C6-N1-C2	-5.25	118.20	120.30
1	A	98	G	C8-N9-C4	-5.22	104.31	106.40
1	A	1042	G	O4'-C1'-N9	5.18	112.34	108.20
24	X	46	G	C5-C6-O6	-5.17	125.50	128.60
1	A	1531	A	O4'-C1'-N9	-5.17	104.06	108.20
1	A	1150	U	C2-N3-C4	5.07	130.04	127.00
24	X	14	A	N1-C6-N6	5.07	121.64	118.60
1	A	1502	A	C5-N7-C8	-5.07	101.36	103.90
1	A	1065	U	P-O3'-C3'	5.04	125.75	119.70
1	A	1278	U	C6-N1-C2	-5.01	117.99	121.00
1	A	748	C	P-O3'-C3'	5.00	125.71	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	231	GLU	Peptide
7	G	78	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	32205	0	16255	428	0
2	B	1846	0	1867	70	0
3	C	1552	0	1546	45	0
4	D	1659	0	1676	53	0
5	E	1129	0	1185	33	0
6	F	806	0	793	17	0
7	G	1231	0	1238	22	0
8	H	1088	0	1126	32	0
9	I	983	0	986	28	0
10	J	709	0	650	32	0
11	K	829	0	825	15	0
12	L	930	0	980	18	0
13	M	958	0	1002	24	0
14	N	492	0	529	20	0
15	O	728	0	760	18	0
16	P	681	0	697	21	0
17	Q	823	0	891	16	0
18	R	555	0	618	12	0
19	S	652	0	662	30	0
20	T	728	0	798	19	0
21	U	199	0	208	5	0
22	V	277	0	140	2	0
23	W	1588	0	820	29	0
23	Y	1581	0	805	56	0
24	X	1625	0	828	9	0
25	A	230	0	0	0	0
25	D	1	0	0	0	0
25	E	1	0	0	0	0
25	F	1	0	0	0	0
25	K	2	0	0	0	0
25	M	1	0	0	0	0
25	N	1	0	0	0	0
25	V	1	0	0	0	0
25	W	7	0	0	0	0
25	X	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Y	3	0	0	0	0
26	A	40	0	37	7	0
27	D	8	0	0	0	0
28	N	1	0	0	0	0
29	X	1	0	0	0	0
30	A	226	0	0	17	0
30	E	3	0	0	0	0
30	J	1	0	0	0	0
30	L	4	0	0	1	0
30	M	1	0	0	0	0
30	V	4	0	0	0	0
30	W	6	0	0	0	0
30	X	8	0	0	0	0
30	Y	3	0	0	0	0
All	All	56420	0	37922	934	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 10.

All (934) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1025:U:O2	1:A:1036:G:O6	1.82	0.98
23:Y:2:C:H42	23:Y:71:G:H1	1.15	0.94
23:Y:51:U:H3	23:Y:63:G:H1	0.97	0.93
23:Y:19:G:N2	23:Y:56:C:N3	2.20	0.90
23:Y:26:A:H61	23:Y:44:G:H1	0.96	0.89
2:B:16:HIS:HB2	2:B:204:ASN:HB3	1.54	0.89
23:Y:26:A:N6	23:Y:44:G:H1	1.69	0.89
7:G:50:ILE:HD11	7:G:58:PRO:HA	1.55	0.89
1:A:266:G:H5''	1:A:268:C:H41	1.37	0.88
1:A:376:G:H5''	16:P:5:ARG:HG2	1.54	0.88
1:A:1502:A:H2	1:A:1505:G:H1	1.19	0.88
1:A:1025:U:H3	1:A:1036:G:H1	1.24	0.85
19:S:20:LEU:HD23	19:S:23:ASN:HD22	1.43	0.83
1:A:1086:U:H3	1:A:1099:G:H22	1.23	0.82
23:Y:2:C:N4	23:Y:71:G:H1	1.78	0.81
1:A:1004:A:N7	1:A:1036:G:N2	2.28	0.81
1:A:1158:C:H5	1:A:1181:G:H1	1.28	0.81
1:A:1314:C:OP2	19:S:4:SER:OG	1.97	0.81
8:H:41:ARG:NH2	8:H:123:GLU:OE2	2.15	0.80
1:A:1182:G:H4'	1:A:1183:A:H5'	1.61	0.80
23:Y:2:C:N3	23:Y:71:G:N2	2.30	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1008:C:N3	1:A:1021:G:O6	2.16	0.79
1:A:1503:A:O2'	22:V:13:A:N1	2.16	0.79
1:A:160:A:N6	1:A:345:C:OP2	2.15	0.78
2:B:155:LEU:HD21	2:B:159:PRO:HG3	1.65	0.77
9:I:50:LEU:HD13	9:I:56:LEU:HA	1.67	0.77
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.15	0.77
1:A:1108:G:O6	30:A:4156:HOH:O	2.03	0.77
8:H:34:GLU:OE1	8:H:37:ARG:NH1	2.17	0.77
1:A:975:A:H4'	1:A:976:G:H5''	1.66	0.76
23:Y:50:U:H3	23:Y:64:A:H2	1.31	0.76
20:T:10:LEU:HB3	20:T:12:ALA:H	1.49	0.76
2:B:69:LEU:HB3	2:B:162:ILE:HG22	1.68	0.75
1:A:201:C:H42	1:A:216:G:H1	1.35	0.74
2:B:33:TYR:HB2	2:B:43:ASP:HB2	1.66	0.74
1:A:406:G:H5'	4:D:5:ILE:HD11	1.69	0.74
2:B:16:HIS:CD2	2:B:17:PHE:H	2.05	0.74
1:A:1069:C:OP2	30:A:4012:HOH:O	2.05	0.73
23:Y:26:A:N1	23:Y:44:G:N2	2.35	0.73
1:A:742:G:OP2	15:O:35:ARG:NH2	2.22	0.73
1:A:677:U:H3	1:A:713:G:H22	1.36	0.73
12:L:71:PRO:O	12:L:102:ARG:NH1	2.21	0.72
1:A:1183:A:O2'	1:A:1184:G:OP1	2.08	0.72
1:A:664:G:H22	1:A:741:G:H1	1.38	0.72
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.71	0.72
23:Y:8:4SU:H4'	23:Y:48:C:H4'	1.72	0.72
17:Q:26:GLN:HG2	17:Q:37:LYS:HG2	1.70	0.71
1:A:1030(C):G:N7	1:A:1031:G:N2	2.38	0.71
3:C:6:HIS:HD2	3:C:8:ILE:H	1.36	0.71
11:K:79:SER:HA	11:K:104:GLN:HB2	1.71	0.70
26:A:3231:PCY:N2	26:A:3231:PCY:O19	2.24	0.70
3:C:78:GLY:HA3	3:C:83:ARG:H	1.56	0.70
5:E:85:GLY:O	5:E:87:SER:N	2.24	0.70
3:C:150:LYS:HE2	3:C:152:ILE:HD11	1.71	0.69
9:I:16:ARG:HB2	9:I:64:THR:HB	1.74	0.69
1:A:1353:G:OP1	21:U:10:ARG:NH1	2.25	0.69
1:A:538:G:H5''	12:L:114:LYS:HB2	1.73	0.69
19:S:63:THR:OG1	19:S:65:ASN:ND2	2.25	0.69
1:A:1129:C:H5''	9:I:16:ARG:HH12	1.57	0.69
1:A:836:G:OP1	18:R:61:LYS:NZ	2.23	0.69
1:A:812:C:N3	30:A:4050:HOH:O	2.25	0.69
1:A:922:G:H4'	5:E:20:GLN:HA	1.75	0.69
23:Y:19:G:N1	23:Y:56:C:N4	2.38	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:67:C:H2'	23:Y:68:C:C6	2.28	0.69
1:A:200:G:H1	1:A:217:C:H42	1.40	0.68
1:A:539:A:OP2	12:L:115:LYS:NZ	2.26	0.68
23:Y:44:G:O2'	23:Y:45:U:OP1	2.10	0.68
1:A:1034:G:H2'	1:A:1035:A:C8	2.27	0.68
1:A:44:G:O6	30:A:4055:HOH:O	2.09	0.68
1:A:1151:A:HO2'	1:A:1152:A:H8	1.41	0.68
10:J:30:SER:O	10:J:81:THR:OG1	2.11	0.68
12:L:49:ASN:ND2	12:L:92:ASP:OD2	2.22	0.68
1:A:972:C:O2'	10:J:55:LYS:O	2.10	0.68
23:Y:50:U:O4	23:Y:64:A:N1	2.27	0.68
1:A:1297:C:O2'	7:G:114:ARG:NH2	2.27	0.68
4:D:173:TRP:CE3	4:D:174:LEU:HG	2.29	0.67
1:A:1352:C:OP1	21:U:3:LYS:NZ	2.23	0.67
19:S:41:VAL:HG12	19:S:43:GLU:H	1.60	0.67
9:I:20:ARG:O	9:I:60:ASP:N	2.23	0.67
1:A:1416:G:N7	30:A:4106:HOH:O	2.28	0.67
1:A:1392:G:N2	1:A:1502:A:H8	1.94	0.66
1:A:572:A:OP1	30:A:4102:HOH:O	2.12	0.66
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.27	0.66
1:A:1238:A:OP2	30:A:4145:HOH:O	2.12	0.66
1:A:953:G:H5'	1:A:965:A:H61	1.60	0.66
1:A:1255:G:OP1	10:J:45:ARG:NH2	2.29	0.66
1:A:1025:U:O2'	1:A:1026:G:O4'	2.14	0.66
9:I:17:VAL:HG23	9:I:63:ILE:HG12	1.78	0.66
23:W:51:U:H2'	23:W:52:G:C8	2.30	0.66
1:A:310:G:OP2	16:P:27:LYS:NZ	2.27	0.66
2:B:47:THR:HA	2:B:202:PRO:HG2	1.77	0.66
1:A:1392:G:H21	1:A:1502:A:H8	1.45	0.65
4:D:15:GLU:HG2	4:D:63:LYS:HB3	1.78	0.65
1:A:1530:G:H2'	1:A:1531:A:O4'	1.96	0.65
1:A:427:U:OP1	4:D:13:ARG:NH2	2.29	0.65
1:A:656:C:O2'	15:O:28:GLN:NE2	2.30	0.65
1:A:76:C:N3	1:A:93:G:O6	2.29	0.65
23:W:19:G:N2	23:W:56:C:N3	2.44	0.65
5:E:33:VAL:HG21	5:E:109:ILE:HA	1.77	0.65
1:A:1002:G:H3'	1:A:1003:G:O4'	1.97	0.65
1:A:837:G:H1	1:A:849:C:H42	1.45	0.65
12:L:24:VAL:HG11	12:L:27:LEU:HD22	1.78	0.65
2:B:201:ILE:HG21	2:B:214:ILE:HG21	1.80	0.64
1:A:78:G:N2	1:A:91:C:N3	2.46	0.64
1:A:1136:U:H5''	1:A:1137:C:C4	2.31	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.79	0.64
9:I:53:VAL:O	9:I:55:ALA:N	2.31	0.64
1:A:1456:G:O3'	20:T:39:LYS:NZ	2.30	0.64
1:A:1008:C:O2	1:A:1021:G:N1	2.27	0.64
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.27	0.64
1:A:97:G:O2'	1:A:98:G:O4'	2.14	0.64
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.79	0.64
12:L:34:ARG:NH2	30:L:201:HOH:O	2.30	0.64
1:A:352:C:OP2	30:A:4109:HOH:O	2.15	0.64
4:D:177:ASP:HB3	4:D:182:LYS:HG2	1.78	0.64
1:A:1183:A:H3'	1:A:1184:G:H5''	1.80	0.63
23:W:19:G:H1	23:W:56:C:H42	1.43	0.63
1:A:812:C:O2	30:A:4048:HOH:O	2.14	0.63
16:P:22:THR:HA	16:P:33:ILE:HG13	1.80	0.63
1:A:159:G:N2	1:A:162:A:OP2	2.32	0.63
1:A:353:A:H5'	1:A:353:A:H8	1.63	0.63
1:A:545:C:OP1	4:D:61:LYS:NZ	2.31	0.63
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.81	0.63
2:B:118:LEU:HB3	2:B:142:LEU:HD12	1.79	0.63
1:A:78:G:N1	1:A:91:C:N4	2.47	0.63
1:A:134:A:H61	16:P:25:ARG:NH1	1.97	0.63
23:Y:19:G:H3'	23:Y:20:U:H6	1.64	0.63
10:J:37:PRO:HA	10:J:72:VAL:HG12	1.80	0.62
23:W:7:A:H61	23:W:66:U:H3	1.45	0.62
1:A:1002:G:C4	1:A:1003:G:H1'	2.34	0.62
1:A:1103:C:OP1	2:B:96:ARG:NH2	2.32	0.62
1:A:316:G:OP2	1:A:351:G:O2'	2.17	0.62
1:A:45:U:H2'	1:A:46:G:C8	2.35	0.62
1:A:519:C:OP2	12:L:50:SER:OG	2.17	0.62
7:G:27:ILE:HD12	7:G:40:ALA:HA	1.82	0.62
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.80	0.62
2:B:16:HIS:O	2:B:18:GLY:N	2.32	0.62
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.82	0.62
20:T:57:ARG:HH12	20:T:100:ILE:HD12	1.64	0.62
3:C:3:ASN:N	3:C:3:ASN:OD1	2.33	0.62
7:G:111:ARG:NH2	7:G:126:ASP:OD2	2.32	0.62
1:A:1435:G:H2'	1:A:1436:U:C6	2.35	0.61
8:H:51:VAL:HG21	8:H:60:ARG:HH11	1.65	0.61
14:N:23:ARG:HH11	14:N:30:ALA:HB2	1.64	0.61
1:A:189(B):C:H42	1:A:189(I):G:H1	1.48	0.61
1:A:452:A:H4'	16:P:72:ARG:NH1	2.15	0.61
2:B:53:ARG:NH2	2:B:198:ASP:O	2.32	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:93:VAL:HG21	2:B:97:TRP:CD1	2.36	0.61
20:T:60:GLU:HG3	20:T:81:LYS:HD2	1.80	0.61
1:A:100:C:H2'	1:A:101:A:C8	2.36	0.61
1:A:1305:G:N2	1:A:1331:G:H1'	2.16	0.61
19:S:32:LYS:HA	19:S:50:ALA:HB3	1.83	0.61
1:A:276:G:O3'	17:Q:68:ARG:NH1	2.33	0.61
2:B:185:ILE:HG22	2:B:199:TYR:HB2	1.83	0.61
3:C:13:GLY:HA3	14:N:57:ARG:NH2	2.16	0.61
23:W:18:G:O2'	23:W:57:G:N2	2.24	0.61
2:B:93:VAL:HG21	2:B:97:TRP:HD1	1.66	0.61
3:C:162:GLN:NE2	22:V:24:A:O2'	2.33	0.61
3:C:8:ILE:HD13	3:C:184:TYR:HB3	1.83	0.61
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.34	0.61
1:A:559:A:OP1	5:E:126:ARG:NH2	2.25	0.61
4:D:128:VAL:N	4:D:131:ARG:O	2.30	0.61
1:A:1381:U:H1'	7:G:79:ARG:HG3	1.83	0.61
23:W:1:G:O6	23:W:72:C:N3	2.34	0.61
1:A:1441:G:H5''	1:A:1442:G:H5'	1.82	0.60
1:A:1442:G:O2'	1:A:1442(A):G:OP1	2.19	0.60
13:M:84:ILE:HG13	13:M:85:GLY:HA2	1.81	0.60
17:Q:76:LEU:HD21	17:Q:79:SER:HB2	1.83	0.60
3:C:12:LEU:HD23	3:C:16:ARG:HB3	1.83	0.60
10:J:26:ALA:O	10:J:84:GLN:NE2	2.34	0.60
1:A:800:G:O6	30:A:4021:HOH:O	2.12	0.60
1:A:976:G:H5'	1:A:1358:U:O2'	2.00	0.60
5:E:151:LEU:HD22	8:H:79:VAL:HG22	1.84	0.60
20:T:43:LEU:O	20:T:47:GLY:N	2.35	0.60
1:A:625:G:H4'	16:P:16:HIS:CD2	2.36	0.59
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.84	0.59
6:F:42:GLU:OE1	6:F:59:TYR:OH	2.13	0.59
14:N:3:ARG:HH21	14:N:3:ARG:HB3	1.66	0.59
4:D:129:ASN:OD1	4:D:145:GLU:N	2.33	0.59
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.84	0.59
12:L:88:GLY:O	12:L:99:HIS:HD2	1.84	0.59
1:A:97:G:O2'	1:A:98:G:H8	1.86	0.59
3:C:57:ILE:HG12	3:C:66:VAL:HG22	1.84	0.59
4:D:155:LEU:HD13	4:D:158:ILE:HD11	1.84	0.59
1:A:1492:A:O2'	1:A:1493:A:O5'	2.10	0.59
1:A:1008:C:N3	1:A:1021:G:C6	2.71	0.58
1:A:1125:U:H4'	10:J:5:ARG:NH2	2.18	0.58
5:E:143:ARG:NH1	8:H:77:GLU:OE1	2.36	0.58
24:X:59:A:H2'	24:X:60:U:H5'	1.83	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:73:ASP:OD1	8:H:75:ARG:HD3	2.03	0.58
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.39	0.58
1:A:997:U:H3	1:A:1044:A:H61	1.51	0.58
1:A:200:G:H1	1:A:217:C:N4	2.02	0.58
9:I:9:ARG:HG2	9:I:14:VAL:HG12	1.86	0.57
1:A:619:U:C2	4:D:135:LEU:HD22	2.40	0.57
1:A:1391:U:H2'	1:A:1392:G:C8	2.40	0.57
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.44	0.57
24:X:21:A:N6	24:X:46:G:H2'	2.19	0.57
1:A:1183:A:HO2'	1:A:1184:G:P	2.27	0.57
23:Y:63:G:H2'	23:Y:64:A:O4'	2.05	0.57
1:A:1191:A:H5''	3:C:4:LYS:NZ	2.20	0.57
15:O:11:VAL:HG21	15:O:34:LEU:HD22	1.86	0.57
1:A:222:U:H2'	1:A:223:U:C6	2.39	0.57
2:B:178:ARG:HG2	8:H:72:PRO:HA	1.85	0.57
10:J:38:ILE:HD11	10:J:71:LEU:HD23	1.87	0.57
23:Y:20:U:H4'	23:Y:21:A:OP1	2.04	0.57
1:A:1510:U:H2'	1:A:1511:G:C8	2.40	0.57
1:A:78:G:C6	1:A:91:C:N4	2.73	0.57
1:A:7:G:O2'	5:E:120:THR:O	2.23	0.57
6:F:97:PHE:N	18:R:30:ASP:OD1	2.37	0.57
1:A:972:C:OP1	30:A:4158:HOH:O	2.18	0.57
1:A:1064:G:H4'	1:A:1065:U:OP1	2.06	0.56
1:A:838:G:H2'	1:A:839:U:H2'	1.86	0.56
1:A:977:A:H1'	1:A:982:U:O4	2.06	0.56
1:A:405:U:OP2	4:D:3:ARG:NH2	2.38	0.56
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.87	0.56
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.85	0.56
23:Y:33:U:H2'	23:Y:35:A:OP2	2.04	0.56
2:B:100:GLY:N	2:B:176:GLU:OE2	2.27	0.56
1:A:1007:C:N3	1:A:1022:G:O6	2.37	0.56
2:B:15:VAL:HG21	2:B:209:ARG:HG2	1.87	0.56
3:C:54:ARG:NH1	3:C:56:ASP:OD2	2.38	0.56
1:A:17:U:H2'	1:A:18:C:C6	2.40	0.56
26:A:3231:PCY:O36	26:A:3231:PCY:O26	2.22	0.56
4:D:108:LEU:HD22	4:D:174:LEU:HD13	1.88	0.56
15:O:64:ARG:HH11	15:O:64:ARG:HB3	1.70	0.56
18:R:56:THR:HB	18:R:58:LEU:HD23	1.87	0.56
23:W:4:C:H2'	23:W:5:G:H8	1.71	0.56
1:A:924:C:O2'	1:A:1502:A:N6	2.37	0.56
23:Y:19:G:H3'	23:Y:20:U:C6	2.39	0.56
13:M:3:ARG:HD2	13:M:9:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:8:4SU:O5'	23:W:8:4SU:H6	2.06	0.56
2:B:16:HIS:CG	2:B:17:PHE:N	2.74	0.55
3:C:17:ASP:O	3:C:54:ARG:NH2	2.40	0.55
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.87	0.55
1:A:60:A:H4'	1:A:61:G:H5'	1.88	0.55
1:A:1392:G:N2	1:A:1502:A:C8	2.74	0.55
1:A:356:A:N3	1:A:368:U:O2'	2.33	0.55
1:A:715:A:H2'	1:A:716:A:C8	2.41	0.55
1:A:975:A:H5'	1:A:975:A:H8	1.70	0.55
9:I:22:GLY:N	9:I:58:HIS:O	2.31	0.55
1:A:165:C:H2'	1:A:166:G:C8	2.42	0.55
1:A:509:A:O2'	1:A:510:A:OP1	2.18	0.55
6:F:91:VAL:HG11	18:R:72:ARG:NH1	2.20	0.55
1:A:1025:U:C2	1:A:1036:G:O6	2.59	0.55
1:A:407:G:OP1	4:D:115:ARG:NH2	2.39	0.55
4:D:190:ASP:HB2	4:D:193:ASP:OD2	2.07	0.55
1:A:1414:U:H3	1:A:1486:G:H1	1.54	0.55
2:B:189:ASP:OD1	2:B:189:ASP:N	2.30	0.55
5:E:91:LEU:HG	5:E:118:ILE:HD11	1.89	0.55
5:E:151:LEU:HD11	8:H:77:GLU:HG2	1.88	0.55
10:J:17:ASP:OD1	10:J:70:ARG:NH1	2.39	0.55
20:T:36:LEU:HD13	20:T:58:LYS:HG3	1.88	0.55
1:A:1007:C:H2'	1:A:1008:C:H5''	1.88	0.54
9:I:21:PRO:HA	9:I:59:PHE:HA	1.90	0.54
1:A:69:G:H2'	1:A:70:G:C8	2.42	0.54
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.89	0.54
3:C:164:ARG:NH1	3:C:166:GLU:OE1	2.40	0.54
24:X:19:G:H4'	24:X:20:U:OP2	2.07	0.54
23:Y:40:C:H2'	23:Y:41:C:H6	1.72	0.54
1:A:153:C:H2'	1:A:154:C:C6	2.42	0.54
1:A:165:C:H2'	1:A:166:G:H8	1.72	0.54
3:C:11:ARG:NH2	3:C:177:THR:O	2.41	0.54
1:A:1112:C:H1'	3:C:179:ARG:HG2	1.88	0.54
1:A:637:G:H2'	1:A:638:G:H8	1.71	0.54
1:A:731:G:H5'	1:A:766:A:H4'	1.89	0.54
1:A:749:C:H2'	1:A:750:G:H8	1.72	0.54
4:D:98:GLU:HG2	4:D:189:PRO:HG2	1.88	0.54
2:B:83:MET:HB3	2:B:234:PRO:HG2	1.88	0.54
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.89	0.54
1:A:376:G:O3'	16:P:5:ARG:HD2	2.07	0.54
1:A:532:A:O2'	1:A:533:A:OP1	2.22	0.54
2:B:162:ILE:O	2:B:185:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:181:ASN:HD21	3:C:204:LEU:HD12	1.73	0.54
4:D:168:ARG:CD	4:D:168:ARG:H	2.21	0.54
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.89	0.54
23:Y:55:PSU:C2	23:Y:57:G:H5'	2.43	0.54
1:A:1218:C:H2'	1:A:1219:U:C6	2.43	0.54
1:A:676:A:H1'	11:K:115:PRO:HB3	1.88	0.54
11:K:99:GLN:HG2	11:K:105:VAL:HG21	1.90	0.53
1:A:134:A:H61	16:P:25:ARG:HH12	1.56	0.53
2:B:178:ARG:HH21	8:H:74:PRO:HB3	1.74	0.53
1:A:110:C:H2'	1:A:111:G:O4'	2.07	0.53
1:A:933:G:O6	7:G:3:ARG:NH2	2.39	0.53
13:M:37:THR:O	13:M:55:ARG:NH1	2.42	0.53
1:A:1001:A:H2'	1:A:1001(A):G:C8	2.43	0.53
1:A:1305:G:H22	1:A:1331:G:H1'	1.72	0.53
4:D:101:LEU:HB2	4:D:138:TYR:HB3	1.90	0.53
1:A:1027:C:N4	1:A:1033:G:O6	2.42	0.53
1:A:1124:G:N7	1:A:1145:C:O2'	2.40	0.53
10:J:5:ARG:NH2	10:J:73:ASP:OD2	2.32	0.53
23:W:4:C:N3	23:W:69:G:O6	2.42	0.53
1:A:1004:A:H5''	1:A:1025:U:C5	2.43	0.53
1:A:954:G:H21	1:A:1227:A:H62	1.56	0.53
9:I:86:VAL:HG13	9:I:96:LEU:HD12	1.91	0.53
23:W:26:A:H61	23:W:44:G:H1	1.55	0.53
23:Y:67:C:H2'	23:Y:68:C:H6	1.71	0.53
1:A:1176:A:H2'	1:A:1177:G:C8	2.43	0.53
15:O:82:ILE:O	15:O:86:GLY:N	2.41	0.53
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.41	0.53
9:I:23:ASN:ND2	9:I:25:LYS:HG2	2.24	0.53
6:F:68:PRO:HB2	6:F:71:ARG:HG3	1.90	0.53
23:Y:40:C:H2'	23:Y:41:C:C6	2.44	0.53
1:A:562:C:H1'	12:L:15:ARG:HB3	1.91	0.53
1:A:78:G:C2	1:A:91:C:N3	2.77	0.53
8:H:112:LEU:HA	8:H:134:ILE:HG12	1.91	0.53
1:A:1149:C:P	9:I:9:ARG:HH21	2.32	0.53
1:A:253:U:OP1	17:Q:67:LYS:NZ	2.42	0.52
1:A:67:C:H2'	1:A:68:G:C8	2.44	0.52
23:W:20:U:H4'	23:W:20:U:OP1	2.07	0.52
4:D:173:TRP:HE1	4:D:193:ASP:HB3	1.74	0.52
20:T:90:GLN:O	20:T:93:GLU:HB3	2.09	0.52
1:A:741:G:H2'	1:A:742:G:O4'	2.09	0.52
2:B:54:THR:HG21	2:B:201:ILE:HD11	1.89	0.52
6:F:45:LEU:HD12	6:F:59:TYR:HD2	1.74	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1179:A:H4'	9:I:103:THR:HA	1.90	0.52
11:K:32:ILE:HG13	11:K:72:ALA:HB2	1.91	0.52
1:A:410:G:OP1	4:D:30:LYS:NZ	2.29	0.52
10:J:35:SER:HB3	10:J:73:ASP:HB2	1.91	0.52
23:Y:18:G:H1	23:Y:55:PSU:H1'	1.74	0.52
3:C:16:ARG:NH2	3:C:183:ASP:OD1	2.36	0.52
1:A:438:G:H4'	4:D:123:HIS:ND1	2.24	0.52
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.92	0.52
1:A:1320:C:O2	19:S:36:ARG:NH2	2.38	0.52
1:A:346:G:C2	1:A:347:G:H1'	2.44	0.52
1:A:347:G:H2'	1:A:348:G:C8	2.44	0.52
1:A:76:C:H2'	1:A:77:G:C8	2.44	0.52
1:A:1158:C:H5	1:A:1181:G:N1	2.02	0.52
1:A:946:A:H2'	1:A:947:G:C8	2.44	0.52
13:M:3:ARG:HG3	13:M:8:GLU:HA	1.92	0.52
18:R:26:LEU:HD23	18:R:29:PHE:CE2	2.45	0.52
1:A:1251:A:H2'	1:A:1252:A:C8	2.45	0.52
1:A:1499:A:H1'	1:A:1520:G:H5'	1.90	0.52
8:H:51:VAL:HG12	8:H:52:ASP:H	1.75	0.52
1:A:189(I):G:H2'	1:A:189(J):G:H5''	1.92	0.52
15:O:26:GLU:OE2	15:O:77:ARG:NE	2.31	0.52
1:A:309:G:O2'	1:A:607:A:N1	2.42	0.51
1:A:250:A:H4'	1:A:251:G:O5'	2.10	0.51
1:A:583:A:OP2	30:A:4025:HOH:O	2.19	0.51
13:M:19:LEU:HD21	13:M:56:LEU:HD11	1.91	0.51
24:X:59:A:C2'	24:X:60:U:H5'	2.40	0.51
1:A:28:G:O2'	1:A:296:U:OP1	2.26	0.51
2:B:77:ALA:HB2	2:B:165:VAL:HG11	1.92	0.51
7:G:48:LYS:O	7:G:52:GLU:HG2	2.11	0.51
20:T:54:LYS:HB2	20:T:100:ILE:HD11	1.93	0.51
1:A:1036:G:H3'	1:A:1037:C:C6	2.45	0.51
9:I:77:ILE:O	9:I:81:ILE:HG22	2.10	0.51
23:Y:34:G:H2'	23:Y:35:A:C8	2.45	0.51
1:A:49:U:O4	1:A:365:U:H5	1.94	0.51
9:I:93:ARG:HB2	9:I:93:ARG:HH11	1.75	0.51
1:A:581:G:OP1	15:O:65:ARG:NH2	2.43	0.51
1:A:757:U:H2'	1:A:758:G:O4'	2.11	0.51
6:F:70:ASP:N	6:F:70:ASP:OD1	2.36	0.51
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.25	0.51
15:O:21:ASP:OD2	15:O:24:SER:HB3	2.10	0.51
16:P:71:ARG:HG3	16:P:80:PHE:HE2	1.75	0.51
1:A:381:C:H2'	1:A:382:A:O4'	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:21:ARG:HH21	2:B:21:ARG:H	1.59	0.51
1:A:1202:G:O4'	14:N:29:ARG:NH1	2.43	0.51
23:W:18:G:N2	23:W:57:G:H2'	2.25	0.51
23:W:18:G:H4'	23:W:60:U:C5	2.46	0.51
1:A:1277:C:O2'	1:A:1279:A:H1'	2.10	0.51
1:A:437:U:H5'	4:D:155:LEU:HD21	1.93	0.51
1:A:1318:A:H5''	19:S:3:ARG:NH1	2.26	0.51
19:S:65:ASN:HD22	19:S:65:ASN:N	2.07	0.51
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.92	0.51
1:A:1001:A:H2'	1:A:1001(A):G:H8	1.76	0.50
1:A:174:C:H2'	1:A:175:C:H6	1.77	0.50
1:A:92:C:H2'	1:A:93:G:C8	2.46	0.50
6:F:33:TYR:CD2	6:F:75:LEU:HD23	2.46	0.50
11:K:84:VAL:HG11	11:K:91:ARG:HD2	1.93	0.50
12:L:117:ARG:HB3	12:L:122:THR:HB	1.93	0.50
13:M:11:ARG:HA	13:M:45:VAL:HB	1.92	0.50
3:C:164:ARG:HG2	3:C:165:THR:H	1.76	0.50
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.76	0.50
26:A:3231:PCY:H40	23:Y:35:A:C2	2.45	0.50
2:B:231:GLU:HB3	2:B:232:PRO:HD3	1.93	0.50
23:Y:6:G:O6	23:Y:7:A:N6	2.45	0.50
9:I:50:LEU:HD23	9:I:81:ILE:HD11	1.94	0.50
1:A:1254:C:H41	10:J:43:ARG:HH12	1.58	0.50
4:D:127:THR:HA	4:D:132:ARG:HA	1.93	0.50
8:H:121:ASP:OD2	8:H:121:ASP:N	2.43	0.50
13:M:88:ARG:HG3	13:M:98:VAL:CG1	2.42	0.50
1:A:93:G:H2'	1:A:96:U:O4'	2.12	0.50
5:E:50:GLU:HB2	5:E:53:LEU:HD13	1.94	0.50
20:T:34:LYS:HZ2	20:T:80:ARG:HH12	1.59	0.50
23:Y:5:G:H1'	23:Y:69:G:N2	2.25	0.50
1:A:1027:C:O2	1:A:1034:G:C2	2.65	0.50
1:A:1027:C:N3	1:A:1034:G:C6	2.80	0.50
1:A:1318:A:H5''	19:S:3:ARG:HH12	1.77	0.50
1:A:69:G:H2'	1:A:70:G:H8	1.76	0.50
1:A:833:U:H2'	1:A:834:C:C6	2.47	0.50
1:A:96:U:O2'	1:A:97:G:H5'	2.11	0.50
1:A:8:A:H5'	5:E:101:ILE:HG22	1.93	0.50
11:K:45:GLY:O	11:K:50:TYR:HB2	2.11	0.50
1:A:21:G:OP1	30:A:4120:HOH:O	2.19	0.50
2:B:109:SER:HA	2:B:112:VAL:HG13	1.94	0.50
1:A:97:G:HO2'	1:A:98:G:H8	1.60	0.50
10:J:11:PHE:HE1	10:J:67:THR:HG22	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1068:G:H8	1:A:1068:G:OP2	1.95	0.49
1:A:1122:U:H2'	1:A:1123:A:O4'	2.12	0.49
1:A:174:C:H2'	1:A:175:C:C6	2.47	0.49
1:A:524:G:H2'	1:A:525:C:C6	2.47	0.49
1:A:590:C:O2	1:A:649:G:N2	2.30	0.49
1:A:922:G:C6	1:A:923:A:C6	3.00	0.49
2:B:231:GLU:HB3	2:B:232:PRO:CD	2.42	0.49
1:A:1060:C:C5	3:C:2:GLY:HA3	2.48	0.49
3:C:87:LEU:O	3:C:91:LEU:N	2.36	0.49
23:W:4:C:H2'	23:W:5:G:C8	2.46	0.49
1:A:1399:C:C2	1:A:1502:A:N6	2.81	0.49
2:B:59:GLU:HB2	2:B:221:LEU:HG	1.94	0.49
2:B:17:PHE:HB2	2:B:44:LEU:HD21	1.94	0.49
19:S:3:ARG:HE	19:S:7:LYS:HB2	1.78	0.49
1:A:1025:U:O2	1:A:1036:G:C6	2.62	0.49
1:A:1034:G:H2'	1:A:1035:A:H8	1.72	0.49
4:D:175:SER:HB3	4:D:186:LEU:HD11	1.93	0.49
5:E:85:GLY:C	5:E:87:SER:H	2.13	0.49
1:A:1066:C:O2'	1:A:1067:A:H5'	2.13	0.49
1:A:131:C:H2'	1:A:132:C:C6	2.48	0.49
3:C:11:ARG:HB3	3:C:15:THR:HB	1.94	0.49
17:Q:62:SER:HB3	17:Q:72:ARG:HD2	1.94	0.49
24:X:8:4SU:O5'	24:X:8:4SU:H6	2.13	0.49
2:B:128:GLU:HB2	2:B:135:GLN:NE2	2.28	0.49
5:E:140:ARG:O	5:E:143:ARG:NH2	2.46	0.49
17:Q:45:HIS:NE2	17:Q:47:PRO:HG3	2.28	0.49
1:A:1244:C:OP1	21:U:9:ARG:HB2	2.13	0.49
1:A:972:C:OP2	10:J:57:LYS:NZ	2.42	0.48
2:B:32:ILE:HD13	2:B:40:HIS:CD2	2.48	0.48
23:Y:48:C:C2	23:Y:59:U:H1'	2.48	0.48
1:A:1236:A:H4'	1:A:1304:G:H4'	1.94	0.48
1:A:346:G:H3'	1:A:347:G:H4'	1.94	0.48
1:A:1298:C:H4'	1:A:1299:A:O4'	2.13	0.48
1:A:347:G:H3'	1:A:348:G:H5''	1.96	0.48
1:A:473:G:H2'	1:A:474:G:H8	1.78	0.48
10:J:11:PHE:HB3	14:N:55:GLY:HA3	1.95	0.48
14:N:6:LEU:HB3	14:N:23:ARG:NH2	2.28	0.48
1:A:447:G:H2'	1:A:485:G:N2	2.28	0.48
1:A:620:C:H2'	1:A:621:A:O4'	2.14	0.48
8:H:82:HIS:N	8:H:138:TRP:O	2.47	0.48
23:W:62:C:H2'	23:W:63:G:H8	1.79	0.48
15:O:5:LYS:HD2	15:O:5:LYS:H	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:33:U:H3'	23:Y:34:G:H5''	1.95	0.48
1:A:1029:C:N3	1:A:1032:G:O6	2.46	0.48
1:A:486:U:H2'	1:A:487:A:H8	1.77	0.48
1:A:628:G:H2'	1:A:629:G:C8	2.49	0.48
13:M:79:LYS:HA	13:M:82:MET:HE2	1.95	0.48
1:A:738:C:H2'	1:A:739:C:H6	1.78	0.48
3:C:18:TRP:HE3	3:C:18:TRP:H	1.60	0.48
7:G:153:HIS:HA	7:G:155:ARG:NH2	2.29	0.48
1:A:1292:U:OP2	7:G:41:ARG:NH2	2.47	0.48
1:A:1062:U:H2'	1:A:1063:C:C6	2.49	0.48
3:C:181:ASN:HD22	3:C:204:LEU:HB2	1.77	0.48
1:A:1053:G:H4'	1:A:1054:C:H5'	1.94	0.48
1:A:486:U:H2'	1:A:487:A:C8	2.49	0.48
7:G:111:ARG:HB3	7:G:113:GLU:OE2	2.14	0.48
10:J:6:ILE:HA	10:J:97:GLU:O	2.14	0.48
19:S:51:VAL:O	19:S:58:VAL:N	2.43	0.48
2:B:95:GLN:HG3	2:B:147:LYS:HD3	1.96	0.48
2:B:60:ASP:O	2:B:64:ARG:HB2	2.14	0.48
7:G:72:ARG:H	7:G:72:ARG:HG2	1.42	0.48
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.95	0.48
1:A:1118:C:H1'	1:A:1179:A:C4	2.49	0.47
1:A:1399:C:H4'	1:A:1400:C:O5'	2.14	0.47
1:A:56:U:H2'	1:A:57:G:C8	2.49	0.47
2:B:115:LEU:O	2:B:119:GLU:HG2	2.14	0.47
3:C:36:ASP:O	3:C:40:ARG:HG3	2.14	0.47
5:E:38:GLN:HB2	5:E:38:GLN:HE21	1.55	0.47
10:J:8:LEU:HD22	10:J:96:ILE:HG12	1.95	0.47
1:A:1057:G:OP2	30:A:4034:HOH:O	2.20	0.47
13:M:11:ARG:C	13:M:13:LYS:H	2.17	0.47
1:A:342:C:C2	1:A:348:G:N2	2.82	0.47
1:A:833:U:H2'	1:A:834:C:H6	1.79	0.47
4:D:166:LYS:HB2	4:D:168:ARG:NH2	2.30	0.47
6:F:69:GLU:O	6:F:72:VAL:HG12	2.14	0.47
1:A:642:A:N3	8:H:113:SER:OG	2.46	0.47
13:M:96:LEU:O	13:M:110:ARG:NH1	2.32	0.47
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.97	0.47
1:A:1370:G:O6	30:A:4100:HOH:O	2.20	0.47
1:A:184:G:H2'	1:A:185:A:C8	2.50	0.47
1:A:625:G:H2'	1:A:626:U:C6	2.50	0.47
12:L:7:ILE:O	12:L:11:VAL:HG23	2.14	0.47
1:A:1004:A:H5''	1:A:1025:U:H5	1.79	0.47
1:A:1029:C:N4	1:A:1030:C:H41	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:6:G:H4'	1:A:298:A:H4'	1.97	0.47
1:A:501:C:H2'	1:A:502:G:C8	2.50	0.47
1:A:695:A:H2'	1:A:696:A:C8	2.49	0.47
1:A:438:G:H4'	4:D:123:HIS:HD1	1.79	0.47
4:D:162:LEU:CD1	4:D:181:MET:HG2	2.45	0.47
4:D:79:PHE:HE1	4:D:204:ILE:HD13	1.80	0.47
1:A:193:C:H2'	1:A:194:C:C6	2.49	0.47
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.96	0.47
10:J:76:ASN:HA	10:J:77:PRO:HD2	1.68	0.47
23:W:7:A:N6	23:W:66:U:H3	2.10	0.47
1:A:164:U:H2'	1:A:165:C:C6	2.50	0.47
1:A:841:U:C5	1:A:848:C:H1'	2.49	0.47
1:A:920:U:H2'	1:A:921:U:C6	2.49	0.47
7:G:152:ALA:O	7:G:155:ARG:HB3	2.15	0.47
19:S:27:GLU:H	19:S:27:GLU:CD	2.18	0.47
20:T:77:ALA:O	20:T:81:LYS:HG3	2.14	0.47
23:Y:54:5MU:O2	23:Y:58:A:N7	2.48	0.47
2:B:61:LEU:HD23	2:B:68:ILE:HD11	1.97	0.47
18:R:38:GLU:HA	18:R:41:LYS:HD2	1.97	0.47
23:W:51:U:H2'	23:W:52:G:H8	1.75	0.47
23:Y:2:C:N4	23:Y:71:G:N1	2.39	0.47
1:A:1028:C:H2'	1:A:1029:C:H4'	1.97	0.47
1:A:748:C:H4'	1:A:749:C:O5'	2.15	0.47
2:B:145:LEU:O	2:B:149:LEU:HB2	2.14	0.47
6:F:75:LEU:O	6:F:79:LEU:HG	2.15	0.47
13:M:11:ARG:O	13:M:13:LYS:N	2.46	0.47
1:A:473:G:H2'	1:A:474:G:C8	2.50	0.46
1:A:1356:G:H2'	1:A:1357:A:C8	2.49	0.46
1:A:662:G:H2'	1:A:663:A:C8	2.49	0.46
2:B:32:ILE:HG21	2:B:40:HIS:HD2	1.79	0.46
4:D:133:VAL:HG12	4:D:135:LEU:H	1.79	0.46
16:P:19:ILE:HG22	16:P:37:GLY:C	2.36	0.46
1:A:76:C:O2	1:A:93:G:N1	2.32	0.46
2:B:62:ALA:HB3	2:B:225:ALA:HB3	1.97	0.46
8:H:39:LEU:HB3	8:H:45:ILE:HG12	1.96	0.46
1:A:376:G:P	16:P:67:THR:HG21	2.56	0.46
1:A:236:G:H5''	17:Q:42:TYR:OH	2.15	0.46
24:X:8:4SU:O2	24:X:21:A:H2	1.98	0.46
23:Y:19:G:H1	23:Y:56:C:N4	2.09	0.46
19:S:3:ARG:HH21	19:S:7:LYS:HB3	1.79	0.46
23:Y:3:C:H42	23:Y:70:G:H1	1.64	0.46
1:A:870:U:H4'	1:A:871:U:H5''	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:121:LYS:HG3	5:E:123:LEU:HG	1.98	0.46
12:L:84:LEU:HB2	12:L:105:TYR:CE2	2.50	0.46
1:A:1278:U:H3'	1:A:1278:U:H6	1.81	0.46
1:A:202:U:O2'	1:A:203:U:O5'	2.29	0.46
1:A:614:A:H2'	1:A:615:C:O4'	2.15	0.46
2:B:16:HIS:CG	2:B:17:PHE:H	2.30	0.46
4:D:53:ASP:O	4:D:57:ARG:HG3	2.16	0.46
9:I:4:TYR:CE1	9:I:88:TYR:HD1	2.34	0.46
1:A:189(D):C:H2'	1:A:189(E):U:O4'	2.16	0.46
1:A:345:C:H6	1:A:345:C:O5'	1.98	0.46
2:B:17:PHE:CB	2:B:44:LEU:HD21	2.46	0.46
1:A:600:C:H5'	8:H:129:VAL:HA	1.98	0.46
9:I:5:TYR:O	9:I:87:GLN:NE2	2.49	0.46
13:M:65:LYS:NZ	13:M:73:GLU:HG3	2.31	0.46
19:S:80:TYR:CZ	19:S:82:GLY:HA2	2.51	0.46
1:A:184:G:H2'	1:A:185:A:H8	1.81	0.46
12:L:33:ARG:HH11	12:L:62:SER:HB3	1.81	0.46
23:W:2:C:H2'	23:W:3:C:C6	2.51	0.46
23:Y:26:A:N6	23:Y:44:G:N1	2.42	0.46
1:A:1030(D):A:H2'	1:A:1031:G:O4'	2.16	0.46
1:A:573:A:OP2	30:A:4006:HOH:O	2.20	0.46
4:D:98:GLU:O	4:D:103:ASN:ND2	2.48	0.46
8:H:101:PRO:HG3	8:H:133:LEU:HD11	1.98	0.46
15:O:7:GLU:O	15:O:11:VAL:HG23	2.16	0.46
20:T:87:LYS:O	20:T:91:LEU:HG	2.16	0.46
23:W:9:A:O2'	23:W:10:G:N7	2.49	0.46
1:A:197:A:C6	1:A:221:C:H4'	2.51	0.46
1:A:38:G:H22	1:A:397:A:H5''	1.81	0.46
1:A:922:G:H2'	1:A:923:A:C8	2.51	0.46
2:B:166:ASP:OD2	2:B:169:LYS:HB2	2.16	0.46
7:G:113:GLU:HG3	7:G:118:VAL:HG12	1.98	0.46
7:G:15:ASP:OD1	7:G:20:ASP:N	2.40	0.46
20:T:10:LEU:HD13	20:T:12:ALA:HB2	1.98	0.46
26:A:3231:PCY:O21	26:A:3231:PCY:N20	2.49	0.45
1:A:707:C:OP1	11:K:85:ARG:NH1	2.48	0.45
7:G:15:ASP:O	7:G:19:GLY:HA2	2.16	0.45
9:I:49:PRO:HG3	9:I:101:PHE:CD2	2.51	0.45
1:A:204:U:H4'	1:A:216:G:O5'	2.15	0.45
19:S:3:ARG:NH2	19:S:7:LYS:HE2	2.31	0.45
23:Y:28:G:H1	23:Y:42:C:H42	1.64	0.45
1:A:434:U:H2'	1:A:435:C:C6	2.51	0.45
1:A:455:C:H6	1:A:455:C:O5'	2.00	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:738:C:H2'	1:A:739:C:C6	2.50	0.45
2:B:80:ILE:HD13	2:B:211:ILE:HG22	1.98	0.45
3:C:15:THR:HG21	3:C:181:ASN:HA	1.99	0.45
7:G:76:ARG:HB3	7:G:156:TRP:HH2	1.82	0.45
23:Y:48:C:OP1	23:Y:48:C:H2'	2.17	0.45
1:A:872:A:C8	1:A:874:G:C8	3.05	0.45
4:D:164:ALA:O	4:D:168:ARG:HD3	2.16	0.45
23:W:19:G:H1	23:W:56:C:N4	2.10	0.45
1:A:1131:G:C2'	1:A:1132:C:H5'	2.47	0.45
1:A:390:C:H2'	1:A:391:G:C8	2.51	0.45
4:D:23:GLY:HA3	4:D:112:VAL:CG1	2.46	0.45
9:I:121:ARG:NH1	9:I:122:ALA:O	2.50	0.45
17:Q:67:LYS:O	17:Q:68:ARG:HB3	2.16	0.45
1:A:130:A:O2'	1:A:131:C:O5'	2.30	0.45
1:A:626:U:C2	1:A:627:G:C8	3.04	0.45
3:C:121:ALA:O	3:C:125:GLU:HG3	2.17	0.45
3:C:82:GLU:HG2	3:C:85:ARG:NH2	2.32	0.45
4:D:164:ALA:C	4:D:168:ARG:HH11	2.19	0.45
1:A:171:A:H2'	1:A:172:A:C8	2.52	0.45
1:A:277:C:H5''	17:Q:68:ARG:NH2	2.31	0.45
1:A:691:G:H2'	1:A:692:U:C6	2.51	0.45
4:D:157:LEU:HD22	4:D:161:ASN:HD21	1.81	0.45
11:K:20:TYR:CZ	11:K:83:ILE:HD12	2.52	0.45
11:K:34:ASP:HB3	11:K:40:ILE:HD11	1.99	0.45
14:N:6:LEU:HD12	14:N:6:LEU:HA	1.88	0.45
1:A:119:A:H4'	1:A:120:A:C8	2.52	0.45
2:B:103:THR:HA	2:B:180:LEU:HD11	1.99	0.45
2:B:215:LEU:O	2:B:219:VAL:HG23	2.17	0.45
1:A:1002:G:O6	1:A:1003:G:N2	2.50	0.45
1:A:1128:C:H2'	1:A:1129:C:H5'	1.98	0.45
1:A:1145:C:H4'	1:A:1146:A:H5''	1.98	0.45
1:A:149:A:H2'	1:A:150:C:C6	2.52	0.45
23:Y:50:U:N3	23:Y:64:A:C2	2.77	0.45
1:A:345:C:H4'	1:A:346:G:N3	2.31	0.45
1:A:1151:A:O4'	10:J:39:PRO:HB2	2.17	0.45
1:A:1286:A:H2	21:U:18:TYR:OH	2.00	0.45
23:W:37:MIA:H162	23:W:37:MIA:H122	1.87	0.45
1:A:1036:G:H5''	1:A:1037:C:C5	2.52	0.44
1:A:1118:C:H2'	1:A:1119:C:H6	1.82	0.44
1:A:1182:G:C4'	1:A:1183:A:H5'	2.39	0.44
1:A:198:G:H2'	1:A:199:G:H8	1.83	0.44
1:A:1241:G:H2'	1:A:1242:C:C6	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1262:C:H2'	1:A:1263:C:C6	2.53	0.44
1:A:1302:U:OP1	13:M:13:LYS:HE3	2.17	0.44
1:A:262:A:H2'	1:A:263:A:C8	2.52	0.44
1:A:371:G:H2'	1:A:372:C:O4'	2.17	0.44
1:A:673:G:H2'	1:A:674:G:C8	2.52	0.44
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.53	0.44
2:B:178:ARG:HH22	8:H:68:ARG:HH22	1.66	0.44
1:A:1054:C:C4	23:W:34:G:H1'	2.52	0.44
1:A:1016:A:H2'	1:A:1017:G:O4'	2.18	0.44
1:A:161:A:H2'	1:A:162:A:C8	2.52	0.44
1:A:192:U:H2'	1:A:193:C:C6	2.52	0.44
1:A:767:A:H2'	1:A:768:A:O4'	2.17	0.44
1:A:973:G:H3'	1:A:974:A:H5''	1.99	0.44
1:A:98:G:H5'	1:A:99:U:OP2	2.17	0.44
4:D:163:GLU:C	4:D:165:MET:H	2.21	0.44
4:D:168:ARG:NE	4:D:168:ARG:H	2.15	0.44
23:Y:19:G:H4'	23:Y:57:G:H22	1.82	0.44
23:Y:69:G:H2'	23:Y:70:G:O4'	2.17	0.44
1:A:664:G:OP1	18:R:64:ARG:NE	2.46	0.44
2:B:170:GLU:O	2:B:174:VAL:HG23	2.18	0.44
1:A:1270:C:OP2	21:U:24:ARG:NH2	2.51	0.44
1:A:1131:G:O2'	1:A:1132:C:H5'	2.18	0.44
1:A:1169:A:C6	1:A:1170:A:C6	3.06	0.44
1:A:154:C:C2'	1:A:155:C:H5'	2.48	0.44
1:A:257:G:C6	1:A:258:G:C5	3.05	0.44
1:A:1073:U:O2'	2:B:104:ASN:OD1	2.28	0.44
4:D:155:LEU:HB3	4:D:158:ILE:HD11	1.99	0.44
13:M:84:ILE:HD12	19:S:74:PHE:CE2	2.53	0.44
16:P:14:ASN:OD1	16:P:42:ARG:NH2	2.50	0.44
18:R:33:ASP:OD2	18:R:36:ASN:HB2	2.17	0.44
23:W:31:A:H2'	23:W:32:PSU:O4'	2.17	0.44
23:Y:25:C:H2'	23:Y:26:A:H8	1.82	0.44
23:Y:19:G:C2	23:Y:56:C:N3	2.86	0.44
1:A:1124:G:O2'	1:A:1145:C:C4	2.71	0.44
1:A:1226:C:H4'	19:S:80:TYR:OH	2.17	0.44
1:A:376:G:OP2	16:P:67:THR:HG21	2.17	0.44
1:A:652:U:O4	1:A:752:G:O2'	2.24	0.44
1:A:964:A:N3	1:A:969:A:O2'	2.40	0.44
2:B:51:LEU:HD23	2:B:201:ILE:HD12	1.99	0.44
5:E:8:GLU:OE2	5:E:63:ARG:NH2	2.49	0.44
20:T:100:ILE:HB	20:T:101:GLY:H	1.63	0.44
20:T:92:LEU:O	20:T:96:GLY:HA2	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1006:C:H2'	1:A:1007:C:C6	2.53	0.44
1:A:1004:A:H5'	1:A:1024:G:O6	2.17	0.44
1:A:1047:G:H5''	14:N:4:LYS:HD2	2.00	0.44
1:A:555:C:H2'	1:A:556:C:C6	2.53	0.44
6:F:19:LEU:HD21	6:F:59:TYR:CE1	2.53	0.44
19:S:66:MET:HB2	19:S:74:PHE:CZ	2.53	0.44
24:X:20:U:H5''	24:X:21:A:OP2	2.18	0.44
23:Y:9:A:O3'	23:Y:45:U:O2'	2.26	0.44
1:A:1286:A:C8	1:A:1287:A:H4'	2.53	0.44
26:A:3231:PCY:H37	23:Y:34:G:O6	2.17	0.44
1:A:376:G:H5''	16:P:5:ARG:CG	2.38	0.44
8:H:86:ILE:HG13	8:H:133:LEU:HD22	2.00	0.44
13:M:115:LYS:HE2	13:M:115:LYS:HB2	1.84	0.44
1:A:1003:G:C2	1:A:1004:A:N3	2.86	0.44
1:A:1032:G:H2'	1:A:1033:G:C8	2.53	0.44
1:A:1353:G:H2'	1:A:1354:C:H6	1.83	0.44
1:A:840:C:H4'	1:A:841:U:OP1	2.18	0.44
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.99	0.44
1:A:1008:C:H2'	1:A:1009:G:O4'	2.17	0.43
1:A:167:G:H2'	1:A:168:G:H8	1.82	0.43
1:A:736:C:H2'	1:A:737:A:C8	2.53	0.43
3:C:82:GLU:HA	3:C:85:ARG:CZ	2.48	0.43
4:D:170:VAL:CG1	4:D:174:LEU:HB2	2.48	0.43
4:D:174:LEU:HD23	4:D:185:PHE:HA	2.00	0.43
23:Y:34:G:C6	23:Y:35:A:C6	3.06	0.43
23:Y:46:7MG:H2'	23:Y:46:7MG:H81	1.75	0.43
1:A:1129:C:H5''	9:I:16:ARG:NH1	2.29	0.43
1:A:109:A:H2'	1:A:326:G:N2	2.33	0.43
1:A:429:U:H4'	1:A:430:A:O5'	2.18	0.43
1:A:72:C:H2'	1:A:73:G:O4'	2.17	0.43
7:G:65:ALA:O	7:G:69:VAL:HG23	2.17	0.43
10:J:11:PHE:CE1	10:J:67:THR:HG22	2.53	0.43
1:A:532:A:N6	1:A:1206:G:O2'	2.52	0.43
2:B:155:LEU:HD11	2:B:159:PRO:HD3	2.00	0.43
10:J:13:HIS:HB3	10:J:68:HIS:CE1	2.54	0.43
1:A:1317:C:N3	19:S:37:ARG:NH2	2.65	0.43
1:A:159:G:N2	1:A:161:A:H3'	2.33	0.43
1:A:7:G:H5'	1:A:298:A:O4'	2.18	0.43
1:A:44:G:C2	1:A:45:U:H1'	2.53	0.43
8:H:72:PRO:O	8:H:74:PRO:HD3	2.19	0.43
12:L:39:VAL:HG11	12:L:41:ARG:NH1	2.33	0.43
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:48:TRP:HH2	16:P:76:GLN:HE22	1.65	0.43
1:A:1346:A:N6	1:A:1375:A:OP2	2.51	0.43
1:A:1493:A:H5''	1:A:1494:G:OP2	2.19	0.43
1:A:481:G:O2'	1:A:483:C:N4	2.48	0.43
1:A:814:A:H2'	1:A:816:A:H5''	2.00	0.43
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.33	0.43
10:J:40:LEU:HB2	10:J:69:ASN:HB2	2.00	0.43
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.18	0.43
11:K:48:ILE:O	11:K:50:TYR:N	2.46	0.43
19:S:30:LEU:HG	19:S:31:ILE:N	2.33	0.43
1:A:269:C:H2'	1:A:270:A:C8	2.54	0.43
2:B:170:GLU:HB3	2:B:173:ALA:HB3	2.01	0.43
2:B:87:ARG:NE	2:B:233:SER:HB3	2.33	0.43
4:D:107:ARG:HD2	4:D:107:ARG:HA	1.88	0.43
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.91	0.43
8:H:25:ASP:OD1	8:H:60:ARG:HG3	2.18	0.43
1:A:232:G:H1'	1:A:262:A:N1	2.33	0.43
1:A:664:G:N2	1:A:741:G:H1	2.11	0.43
1:A:890:G:O2'	1:A:906:G:O6	2.18	0.43
1:A:936:C:H2'	1:A:937:A:O4'	2.18	0.43
4:D:173:TRP:CZ3	4:D:174:LEU:HG	2.53	0.43
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.99	0.43
13:M:15:VAL:HG22	13:M:43:THR:O	2.18	0.43
1:A:1149:C:H2'	1:A:1150:U:C6	2.53	0.43
1:A:1164:G:H2'	1:A:1165:C:C6	2.53	0.43
1:A:456:C:H2'	1:A:457:C:C6	2.53	0.43
1:A:974:A:H8	1:A:974:A:OP1	2.01	0.43
3:C:19:GLU:HB3	3:C:40:ARG:NH2	2.34	0.43
4:D:99:SER:O	4:D:140:VAL:HG23	2.19	0.43
4:D:157:LEU:HD22	4:D:161:ASN:ND2	2.34	0.43
1:A:1302:U:C5	13:M:17:VAL:HG21	2.53	0.43
23:Y:25:C:H2'	23:Y:26:A:C8	2.54	0.43
23:Y:71:G:H2'	23:Y:72:C:C6	2.54	0.43
1:A:1240:U:O2'	7:G:32:ARG:NH2	2.51	0.43
1:A:1316:G:H22	1:A:1319:A:H5''	1.84	0.43
2:B:196:LEU:HD12	2:B:196:LEU:HA	1.80	0.43
3:C:45:LYS:HG3	3:C:46:GLU:N	2.34	0.43
5:E:145:LYS:O	5:E:149:GLU:HG2	2.19	0.43
13:M:2:ALA:N	13:M:8:GLU:OE1	2.52	0.43
18:R:32:ARG:HA	18:R:69:THR:HG21	2.01	0.43
23:W:62:C:H2'	23:W:63:G:C8	2.54	0.43
1:A:1118:C:H2'	1:A:1119:C:C6	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1315:U:H2'	1:A:1316:G:O4'	2.19	0.43
1:A:411:A:OP2	4:D:30:LYS:HD2	2.19	0.43
11:K:99:GLN:HE21	11:K:108:ILE:HD11	1.83	0.43
15:O:61:GLY:O	15:O:65:ARG:HG3	2.19	0.43
1:A:955:U:O2'	19:S:83:HIS:HD2	2.01	0.43
23:Y:54:5MU:C4	23:Y:55:PSU:C2	3.07	0.43
1:A:113:G:H2'	1:A:114:U:C6	2.54	0.42
1:A:154:C:N3	1:A:168:G:C2	2.87	0.42
1:A:448:A:O5'	1:A:485:G:N2	2.45	0.42
1:A:553:A:H2'	1:A:554:C:C6	2.54	0.42
2:B:73:THR:OG1	2:B:170:GLU:OE1	2.31	0.42
5:E:152:ARG:NH2	8:H:107:LEU:O	2.52	0.42
2:B:178:ARG:HH22	8:H:68:ARG:HH12	1.66	0.42
13:M:84:ILE:HD12	19:S:74:PHE:CZ	2.54	0.42
1:A:1446:U:O2'	1:A:1447:A:O5'	2.37	0.42
1:A:149:A:H2'	1:A:150:C:H6	1.84	0.42
1:A:993:G:H2'	1:A:995:C:H41	1.84	0.42
3:C:35:GLU:CD	3:C:59:ARG:HH22	2.22	0.42
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.54	0.42
13:M:96:LEU:C	13:M:110:ARG:HG2	2.39	0.42
3:C:22:TRP:CZ2	14:N:54:PRO:HG3	2.55	0.42
1:A:1343:G:H2'	1:A:1344:C:C6	2.54	0.42
2:B:88:ALA:O	2:B:226:ARG:NH1	2.52	0.42
2:B:76:GLN:H	2:B:76:GLN:CD	2.21	0.42
6:F:6:VAL:HG13	6:F:90:VAL:HG22	2.01	0.42
13:M:80:ARG:HH21	19:S:69:HIS:HE1	1.66	0.42
15:O:56:LEU:O	15:O:60:VAL:HG23	2.19	0.42
23:Y:51:U:O2	23:Y:63:G:N2	2.47	0.42
1:A:377:G:OP1	16:P:3:LYS:HD2	2.19	0.42
1:A:975:A:H5'	1:A:975:A:C8	2.53	0.42
3:C:142:MET:HG3	3:C:170:GLN:HB3	2.00	0.42
4:D:170:VAL:HG12	4:D:174:LEU:HB2	2.01	0.42
5:E:148:VAL:HG21	8:H:107:LEU:HB3	2.00	0.42
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.19	0.42
15:O:26:GLU:HG2	15:O:26:GLU:H	1.38	0.42
19:S:63:THR:O	19:S:66:MET:HG2	2.18	0.42
1:A:1219:U:OP1	14:N:19:ARG:NH2	2.47	0.42
1:A:922:G:N3	1:A:1398:A:H2	2.18	0.42
4:D:138:TYR:HE1	4:D:140:VAL:HA	1.83	0.42
10:J:70:ARG:HA	10:J:70:ARG:HD3	1.71	0.42
12:L:28:LYS:HE2	12:L:64:TYR:CE1	2.54	0.42
1:A:1030(A):G:O2'	1:A:1030(C):G:N7	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:123:C:OP1	1:A:311:C:O2'	2.32	0.42
1:A:1314:C:H2'	1:A:1315:U:C6	2.54	0.42
1:A:598:U:O4	30:A:4079:HOH:O	2.21	0.42
2:B:211:ILE:HG22	2:B:215:LEU:HD12	2.00	0.42
10:J:45:ARG:HG2	10:J:47:PHE:CZ	2.55	0.42
16:P:20:VAL:HG21	16:P:32:TYR:CD2	2.55	0.42
1:A:1169:A:H2'	1:A:1170:A:C8	2.54	0.42
1:A:1316:G:N1	1:A:1319:A:OP2	2.49	0.42
1:A:262:A:C6	1:A:263:A:C6	3.08	0.42
1:A:757:U:O2'	1:A:879:C:O2	2.34	0.42
2:B:69:LEU:HD12	2:B:91:PRO:O	2.19	0.42
4:D:188:LEU:HA	4:D:189:PRO:HD3	1.85	0.42
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.84	0.42
19:S:36:ARG:HB3	19:S:72:GLY:HA3	2.02	0.42
1:A:1118:C:H1'	1:A:1179:A:C5	2.54	0.42
1:A:918:A:H2'	1:A:919:A:O4'	2.19	0.42
5:E:145:LYS:HB3	5:E:145:LYS:HE2	1.82	0.42
18:R:47:THR:HG23	18:R:49:LYS:HG3	2.02	0.42
20:T:13:LEU:HD12	20:T:14:LYS:N	2.35	0.42
1:A:1002:G:C5	1:A:1003:G:H1'	2.54	0.42
1:A:1530:G:H4'	1:A:1530:G:OP1	2.19	0.42
1:A:501:C:H2'	1:A:502:G:H8	1.84	0.42
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.60	0.42
1:A:1291:G:O2'	9:I:38:GLN:OE1	2.30	0.42
1:A:107:G:H2'	1:A:108:G:O4'	2.20	0.42
1:A:431:A:H2'	1:A:432:A:O4'	2.20	0.42
2:B:220:ASP:O	2:B:224:GLN:HG3	2.20	0.42
2:B:230:VAL:HG22	2:B:231:GLU:H	1.84	0.42
3:C:6:HIS:CD2	3:C:8:ILE:H	2.27	0.42
8:H:29:SER:HB3	8:H:32:LYS:HG3	2.02	0.42
1:A:130:A:H5'	17:Q:63:ARG:NE	2.35	0.42
1:A:1106:G:C6	1:A:1107:C:C4	3.08	0.41
1:A:31:G:O2'	1:A:48:C:N4	2.53	0.41
1:A:50:A:H1'	1:A:52:G:C8	2.55	0.41
2:B:133:LYS:O	2:B:137:ARG:HG3	2.19	0.41
5:E:36:ASP:OD1	5:E:38:GLN:N	2.41	0.41
5:E:41:VAL:HG11	5:E:109:ILE:O	2.20	0.41
8:H:19:VAL:HG23	8:H:21:LYS:HD3	2.02	0.41
8:H:56:LYS:HA	8:H:56:LYS:HD3	1.87	0.41
1:A:1368:G:OP2	9:I:112:LYS:HG3	2.19	0.41
10:J:90:LEU:HA	10:J:91:PRO:HD3	1.95	0.41
11:K:81:ASP:OD1	11:K:107:SER:OG	2.25	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:92:ASP:O	12:L:94:PRO:HD3	2.19	0.41
20:T:48:LYS:HD3	20:T:48:LYS:HA	1.85	0.41
23:W:26:A:N6	23:W:44:G:H1	2.18	0.41
1:A:1292:U:H5'	9:I:38:GLN:OE1	2.19	0.41
2:B:134:GLU:O	2:B:138:LEU:HG	2.20	0.41
9:I:93:ARG:HB2	9:I:93:ARG:NH1	2.35	0.41
16:P:52:ASP:HB3	16:P:55:ARG:HB2	2.02	0.41
1:A:1022:G:H4'	1:A:1022:G:OP1	2.21	0.41
1:A:1278:U:H5'	1:A:1279:A:C5'	2.50	0.41
1:A:266:G:O2'	1:A:267:C:OP2	2.33	0.41
1:A:92:C:H2'	1:A:93:G:H8	1.84	0.41
3:C:130:VAL:O	3:C:134:ILE:HG13	2.20	0.41
4:D:166:LYS:HB2	4:D:168:ARG:CZ	2.50	0.41
24:X:21:A:H61	24:X:46:G:H2'	1.84	0.41
23:Y:69:G:C2	23:Y:70:G:H1'	2.55	0.41
1:A:1028:C:N3	1:A:1029:C:H1'	2.35	0.41
1:A:601:C:H2'	1:A:602:A:H8	1.84	0.41
1:A:658:G:H2'	1:A:659:U:C6	2.55	0.41
1:A:865:A:H2	1:A:918:A:H4'	1.85	0.41
1:A:911:U:OP1	12:L:95:GLY:HA2	2.20	0.41
5:E:83:GLU:HG2	5:E:88:LYS:HB2	2.02	0.41
7:G:14:PRO:HG3	7:G:21:VAL:HG13	2.02	0.41
1:A:362:G:O3'	12:L:33:ARG:NH2	2.53	0.41
14:N:13:THR:HA	14:N:14:PRO:HD3	1.95	0.41
18:R:59:SER:OG	18:R:62:GLU:HG2	2.20	0.41
23:W:1:G:H2'	23:W:1:G:N3	2.34	0.41
26:A:3231:PCY:H40	23:Y:35:A:N1	2.36	0.41
1:A:1001(A):G:C6	1:A:1002:G:N7	2.89	0.41
1:A:1125:U:H4'	10:J:5:ARG:HH22	1.83	0.41
1:A:892:A:O2'	1:A:1415:G:H4'	2.20	0.41
1:A:1516:G:H2'	1:A:1518:A:OP2	2.21	0.41
1:A:691:G:OP2	11:K:26:ASN:ND2	2.43	0.41
3:C:131:ARG:NE	3:C:166:GLU:OE2	2.53	0.41
3:C:152:ILE:HG23	3:C:167:TRP:HB3	2.02	0.41
1:A:1049:U:OP1	14:N:3:ARG:HB2	2.20	0.41
1:A:1145:C:H4'	1:A:1146:A:C5'	2.51	0.41
4:D:163:GLU:O	4:D:166:LYS:HG2	2.20	0.41
9:I:24:GLY:HA2	9:I:59:PHE:O	2.20	0.41
16:P:27:LYS:HE3	16:P:27:LYS:HB2	1.72	0.41
3:C:148:GLY:HA3	3:C:172:ARG:O	2.20	0.41
5:E:122:GLU:O	5:E:126:ARG:NH1	2.53	0.41
14:N:33:VAL:HA	14:N:40:CYS:HA	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1261:A:H3'	1:A:1262:C:C6	2.56	0.41
1:A:674:G:H2'	1:A:675:A:C8	2.56	0.41
6:F:44:GLY:HA2	6:F:59:TYR:CE2	2.56	0.41
6:F:91:VAL:HG11	18:R:72:ARG:HH12	1.86	0.41
16:P:69:THR:O	16:P:73:LEU:HG	2.21	0.41
17:Q:45:HIS:O	17:Q:73:VAL:HG23	2.21	0.41
20:T:8:ARG:O	20:T:9:ASN:HB2	2.21	0.41
23:Y:64:A:H2'	23:Y:65:G:C8	2.56	0.41
1:A:1261:A:H5''	1:A:1262:C:OP2	2.21	0.41
1:A:189:G:H1	1:A:189(K):U:H3	1.68	0.41
26:A:3231:PCY:H24	26:A:3231:PCY:H17	1.77	0.41
1:A:621:A:H2'	1:A:622:A:C8	2.56	0.41
1:A:974:A:OP2	14:N:29:ARG:NH2	2.53	0.41
2:B:105:PHE:CZ	2:B:155:LEU:HD12	2.56	0.41
2:B:223:ILE:HD12	2:B:230:VAL:HG12	2.03	0.41
1:A:1223:C:P	19:S:78:ARG:HH21	2.43	0.41
23:Y:44:G:H3'	23:Y:45:U:C6	2.56	0.41
1:A:1077:G:N2	1:A:1080:A:OP2	2.45	0.41
1:A:1121:U:H2'	1:A:1122:U:O4'	2.21	0.41
1:A:1191:A:OP1	3:C:4:LYS:NZ	2.45	0.41
1:A:216:G:C2	1:A:217:C:C4	3.08	0.41
1:A:308:C:H2'	1:A:309:G:C8	2.56	0.41
1:A:826:C:H4'	8:H:12:ARG:HG2	2.02	0.41
5:E:110:LEU:HD13	5:E:118:ILE:HD13	2.02	0.41
6:F:2:ARG:HG3	6:F:69:GLU:HG3	2.03	0.41
8:H:49:GLU:HG2	8:H:62:TYR:HE1	1.86	0.41
10:J:35:SER:N	10:J:73:ASP:O	2.38	0.41
13:M:3:ARG:HD3	13:M:4:ILE:HG22	2.02	0.41
1:A:193:C:H2'	1:A:194:C:H6	1.85	0.41
1:A:601:C:H2'	1:A:602:A:C8	2.56	0.41
1:A:61:G:H2'	1:A:62:U:O4'	2.21	0.41
2:B:189:ASP:HB2	2:B:190:THR:H	1.73	0.41
3:C:108:ASN:HB3	3:C:111:LEU:HD12	2.03	0.41
3:C:65:ALA:HA	3:C:100:ALA:HB3	2.03	0.41
4:D:134:ASP:O	4:D:136:PRO:HD3	2.21	0.41
1:A:542:G:H5'	4:D:41:GLY:HA3	2.03	0.41
10:J:35:SER:CB	10:J:73:ASP:HB2	2.49	0.41
19:S:20:LEU:HD23	19:S:23:ASN:ND2	2.23	0.41
20:T:99:LEU:HA	20:T:100:ILE:O	2.21	0.41
1:A:1003:G:O3'	1:A:1004:A:H4'	2.22	0.40
1:A:1263:C:H5''	1:A:1264:C:OP2	2.21	0.40
2:B:19:HIS:HE1	2:B:189:ASP:HB3	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:S:22:LEU:C	19:S:27:GLU:HG3	2.41	0.40
23:W:54:5MU:H73	23:W:55:PSU:O2	2.22	0.40
23:Y:35:A:H2'	23:Y:36:A:C8	2.57	0.40
1:A:1007:C:N3	1:A:1022:G:C6	2.89	0.40
1:A:1128:C:C2'	1:A:1129:C:H5'	2.51	0.40
1:A:179:A:C5	1:A:180:U:C4	3.09	0.40
5:E:105:VAL:HB	5:E:106:PRO:HD3	2.03	0.40
5:E:82:VAL:HG21	5:E:138:ALA:HA	2.03	0.40
10:J:62:HIS:HB3	14:N:59:ALA:HB3	2.03	0.40
19:S:65:ASN:N	19:S:65:ASN:ND2	2.68	0.40
23:W:43:C:H2'	23:W:44:G:C8	2.56	0.40
1:A:1068:G:N2	1:A:1191:A:N3	2.60	0.40
1:A:374:A:C6	1:A:375:U:C4	3.09	0.40
1:A:461:A:O2'	1:A:470:C:H5'	2.22	0.40
1:A:769:G:H4'	1:A:1513:A:H4'	2.04	0.40
4:D:63:LYS:HG3	4:D:64:LEU:H	1.87	0.40
7:G:8:GLU:H	7:G:8:GLU:HG3	1.63	0.40
16:P:4:ILE:HB	16:P:66:PRO:HA	2.03	0.40
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.22	0.40
20:T:10:LEU:HD22	20:T:11:SER:H	1.86	0.40
1:A:1035:A:H2	1:A:1036:G:C5	2.39	0.40
2:B:15:VAL:O	2:B:16:HIS:HB3	2.22	0.40
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.79	0.40
13:M:13:LYS:O	13:M:44:ARG:HA	2.22	0.40
1:A:235:C:H5'	17:Q:70:ARG:HG2	2.03	0.40
23:W:63:G:H2'	23:W:64:A:O4'	2.21	0.40
1:A:1288:A:H2'	1:A:1289:A:C8	2.57	0.40
1:A:355:C:C4	1:A:356:A:N7	2.89	0.40
1:A:580:U:H5''	15:O:58:MET:HG2	2.03	0.40
24:X:4:G:H2'	24:X:5:G:C8	2.55	0.40
23:Y:57:G:H2'	23:Y:57:G:N3	2.35	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%)	200 (87%)	19 (8%)	10 (4%)	4	4
3	C	204/239 (85%)	184 (90%)	17 (8%)	3 (2%)	15	25
4	D	206/209 (99%)	192 (93%)	12 (6%)	2 (1%)	22	37
5	E	146/162 (90%)	134 (92%)	9 (6%)	3 (2%)	11	16
6	F	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	G	153/156 (98%)	143 (94%)	8 (5%)	2 (1%)	18	29
8	H	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	I	125/128 (98%)	111 (89%)	11 (9%)	3 (2%)	9	13
10	J	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	6	7
11	K	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	13	20
12	L	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
13	M	121/126 (96%)	110 (91%)	9 (7%)	2 (2%)	14	21
14	N	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
15	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	P	80/88 (91%)	78 (98%)	2 (2%)	0	100	100
17	Q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
18	R	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
19	S	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
20	T	94/106 (89%)	84 (89%)	3 (3%)	7 (7%)	2	1
21	U	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	2327/2538 (92%)	2147 (92%)	143 (6%)	37 (2%)	14	23

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	126	GLU
2	B	231	GLU
3	C	65	ALA
9	I	44	VAL

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Mol	Chain	Res	Type
9	I	54	ASP
10	J	77	PRO
20	T	47	GLY
3	C	66	VAL
5	E	85	GLY
5	E	86	ALA
9	I	43	ALA
10	J	31	GLY
10	J	91	PRO
11	K	49	GLY
2	B	150	SER
4	D	166	LYS
4	D	173	TRP
13	M	12	ASN
20	T	9	ASN
20	T	10	LEU
20	T	94	ALA
20	T	100	ILE
20	T	102	GLY
2	B	10	LEU
3	C	107	GLN
5	E	69	VAL
7	G	80	VAL
13	M	11	ARG
2	B	124	SER
11	K	105	VAL
20	T	95	ALA
2	B	202	PRO
7	G	17	VAL

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	192/220 (87%)	169 (88%)	23 (12%)	7	12
3	C	143/188 (76%)	132 (92%)	11 (8%)	18	32
4	D	170/181 (94%)	155 (91%)	15 (9%)	14	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	113/123 (92%)	106 (94%)	7 (6%)	26	43
6	F	83/90 (92%)	77 (93%)	6 (7%)	21	35
7	G	119/127 (94%)	106 (89%)	13 (11%)	9	15
8	H	114/119 (96%)	107 (94%)	7 (6%)	26	44
9	I	90/99 (91%)	82 (91%)	8 (9%)	14	25
10	J	66/92 (72%)	62 (94%)	4 (6%)	26	44
11	K	82/99 (83%)	76 (93%)	6 (7%)	20	35
12	L	97/109 (89%)	93 (96%)	4 (4%)	41	66
13	M	93/101 (92%)	83 (89%)	10 (11%)	9	16
14	N	49/50 (98%)	43 (88%)	6 (12%)	7	12
15	O	78/80 (98%)	67 (86%)	11 (14%)	5	8
16	P	69/74 (93%)	62 (90%)	7 (10%)	11	19
17	Q	94/97 (97%)	91 (97%)	3 (3%)	51	77
18	R	59/77 (77%)	56 (95%)	3 (5%)	33	55
19	S	69/80 (86%)	66 (96%)	3 (4%)	40	64
20	T	70/82 (85%)	64 (91%)	6 (9%)	15	26
21	U	18/22 (82%)	16 (89%)	2 (11%)	9	15
All	All	1868/2110 (88%)	1713 (92%)	155 (8%)	16	28

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	11	LEU
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	24	TRP
2	B	64	ARG
2	B	76	GLN
2	B	94	ASN
2	B	114	ARG
2	B	127	ILE
2	B	144	ARG
2	B	145	LEU

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Mol	Chain	Res	Type
2	B	155	LEU
2	B	157	ARG
2	B	189	ASP
2	B	196	LEU
2	B	200	ILE
2	B	209	ARG
2	B	213	LEU
2	B	217	ARG
2	B	221	LEU
3	C	3	ASN
3	C	8	ILE
3	C	21	ARG
3	C	28	GLN
3	C	37	GLN
3	C	40	ARG
3	C	45	LYS
3	C	89	GLU
3	C	119	ARG
3	C	131	ARG
3	C	150	LYS
4	D	5	ILE
4	D	15	GLU
4	D	19	LEU
4	D	31	CYS
4	D	49	ARG
4	D	58	LEU
4	D	115	ARG
4	D	127	THR
4	D	135	LEU
4	D	140	VAL
4	D	141	ARG
4	D	150	GLU
4	D	157	LEU
4	D	158	ILE
4	D	168	ARG
5	E	31	LEU
5	E	38	GLN
5	E	41	VAL
5	E	47	LYS
5	E	51	VAL
5	E	73	ASN
5	E	151	LEU

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Mol	Chain	Res	Type
6	F	36	ARG
6	F	55	ASP
6	F	70	ASP
6	F	74	ASP
6	F	75	LEU
6	F	82	ARG
7	G	8	GLU
7	G	13	GLN
7	G	50	ILE
7	G	51	GLN
7	G	52	GLU
7	G	72	ARG
7	G	76	ARG
7	G	79	ARG
7	G	104	LEU
7	G	113	GLU
7	G	114	ARG
7	G	138	LYS
7	G	155	ARG
8	H	21	LYS
8	H	52	ASP
8	H	75	ARG
8	H	78	GLN
8	H	91	ARG
8	H	95	VAL
8	H	97	VAL
9	I	14	VAL
9	I	23	ASN
9	I	65	VAL
9	I	86	VAL
9	I	89	ASN
9	I	108	VAL
9	I	127	LYS
9	I	128	ARG
10	J	5	ARG
10	J	23	ILE
10	J	55	LYS
10	J	84	GLN
11	K	16	SER
11	K	31	THR
11	K	48	ILE
11	K	96	ARG

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Mol	Chain	Res	Type
11	K	104	GLN
11	K	114	VAL
12	L	24	VAL
12	L	33	ARG
12	L	53	ARG
12	L	60	LEU
13	M	3	ARG
13	M	4	ILE
13	M	15	VAL
13	M	19	LEU
13	M	43	THR
13	M	56	LEU
13	M	70	LEU
13	M	73	GLU
13	M	102	ARG
13	M	110	ARG
14	N	3	ARG
14	N	7	ILE
14	N	18	VAL
14	N	23	ARG
14	N	33	VAL
14	N	50	LYS
15	O	3	ILE
15	O	5	LYS
15	O	22	THR
15	O	24	SER
15	O	26	GLU
15	O	38	ARG
15	O	39	LEU
15	O	41	GLU
15	O	47	LYS
15	O	64	ARG
15	O	76	GLU
16	P	19	ILE
16	P	20	VAL
16	P	27	LYS
16	P	50	LYS
16	P	54	GLU
16	P	60	LEU
16	P	62	VAL
17	Q	14	LYS
17	Q	74	LEU

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Mol	Chain	Res	Type
17	Q	83	ASP
18	R	31	LEU
18	R	46	GLU
18	R	76	LEU
19	S	28	LYS
19	S	37	ARG
19	S	65	ASN
20	T	8	ARG
20	T	13	LEU
20	T	30	LYS
20	T	45	GLN
20	T	56	MET
20	T	62	LEU
21	U	9	ARG
21	U	10	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	16	HIS
2	B	19	HIS
2	B	40	HIS
2	B	94	ASN
3	C	6	HIS
3	C	28	GLN
3	C	37	GLN
3	C	98	ASN
3	C	102	ASN
3	C	104	GLN
3	C	123	GLN
3	C	136	GLN
3	C	162	GLN
3	C	181	ASN
4	D	45	GLN
4	D	77	ASN
4	D	125	HIS
5	E	38	GLN
5	E	141	GLN
6	F	100	ASN
7	G	28	ASN
7	G	97	GLN
9	I	23	ASN

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Mol	Chain	Res	Type
9	I	58	HIS
10	J	56	HIS
11	K	99	GLN
11	K	104	GLN
12	L	78	GLN
12	L	99	HIS
15	O	28	GLN
15	O	53	HIS
17	Q	16	GLN
19	S	23	ASN
19	S	65	ASN
19	S	69	HIS
19	S	83	HIS
20	T	42	GLN
20	T	45	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1495/1521 (98%)	306 (20%)	21 (1%)
22	V	12/24 (50%)	3 (25%)	0
23	W	71/76 (93%)	30 (42%)	2 (2%)
23	Y	71/76 (93%)	33 (46%)	1 (1%)
24	X	75/77 (97%)	18 (24%)	1 (1%)
All	All	1724/1774 (97%)	390 (22%)	25 (1%)

All (390) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	54	C
1	A	61	G
1	A	65	U
1	A	70	G

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Mol	Chain	Res	Type
1	A	73	G
1	A	78	G
1	A	79	G
1	A	96	U
1	A	97	G
1	A	98	G
1	A	111	G
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	131	C
1	A	145	G
1	A	146	G
1	A	155	C
1	A	156	G
1	A	163	C
1	A	166	G
1	A	171	A
1	A	174	C
1	A	180	U
1	A	182	U
1	A	189(C)	C
1	A	189(E)	U
1	A	189(F)	U
1	A	189(I)	G
1	A	189(J)	G
1	A	189(K)	U
1	A	190	U
1	A	194	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	217	C
1	A	220	G
1	A	247	G
1	A	251	G
1	A	253	U
1	A	258	G

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Mol	Chain	Res	Type
1	A	262	A
1	A	266	G
1	A	267	C
1	A	289	G
1	A	301	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	341	C
1	A	346	G
1	A	347	G
1	A	348	G
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	382	A
1	A	384	G
1	A	388	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	442	C
1	A	443	C
1	A	449	C
1	A	452	A
1	A	455	C
1	A	457	C
1	A	461	A
1	A	470	C
1	A	475	G
1	A	477	A

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Mol	Chain	Res	Type
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	513	C
1	A	518	C
1	A	521	G
1	A	524	G
1	A	527	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	581	G
1	A	590	C
1	A	596	C
1	A	619	U
1	A	630	G
1	A	653	A
1	A	657	G
1	A	660	G
1	A	665	A
1	A	671	G
1	A	673	G
1	A	687	A
1	A	688	G
1	A	693	G
1	A	695	A
1	A	703	G
1	A	723	U
1	A	731	G
1	A	733	A

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Mol	Chain	Res	Type
1	A	749	C
1	A	752	G
1	A	755	G
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	817	C
1	A	821	G
1	A	827	U
1	A	828	A
1	A	829	G
1	A	833	U
1	A	834	C
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	853	G
1	A	859	A
1	A	874	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	960	U
1	A	961	U
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	991	U
1	A	992	U
1	A	993	G

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Mol	Chain	Res	Type
1	A	996	A
1	A	997	U
1	A	998	G
1	A	1003	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1008	C
1	A	1014	A
1	A	1020	U
1	A	1021	G
1	A	1022	G
1	A	1023	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1029	C
1	A	1030(A)	G
1	A	1030(C)	G
1	A	1030(D)	A
1	A	1031	G
1	A	1033	G
1	A	1035	A
1	A	1037	C
1	A	1039	C
1	A	1054	C
1	A	1060	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1076	C
1	A	1081	G
1	A	1088	G
1	A	1089	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1104	G
1	A	1108	G
1	A	1110	A

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Mol	Chain	Res	Type
1	A	1122	U
1	A	1123	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1130	A
1	A	1132	C
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	1145	C
1	A	1146	A
1	A	1152	A
1	A	1154	G
1	A	1157	A
1	A	1158	C
1	A	1159	U
1	A	1175	G
1	A	1183	A
1	A	1184	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1227	A
1	A	1228	C
1	A	1236	A
1	A	1238	A
1	A	1250	A
1	A	1255	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1263	C
1	A	1270	C

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Mol	Chain	Res	Type
1	A	1272	G
1	A	1273	G
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1297	C
1	A	1299	A
1	A	1300	G
1	A	1302	U
1	A	1317	C
1	A	1319	A
1	A	1320	C
1	A	1338	G
1	A	1340	A
1	A	1346	A
1	A	1347	G
1	A	1358	U
1	A	1363	C
1	A	1370	G
1	A	1397	C
1	A	1419	G
1	A	1442	G
1	A	1442(A)	G
1	A	1442(B)	A
1	A	1446	U
1	A	1447	A
1	A	1452	C
1	A	1456	G
1	A	1492	A
1	A	1493	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

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Mol	Chain	Res	Type
22	V	13	A
22	V	14	A
22	V	24	A
23	W	2	C
23	W	3	C
23	W	6	G
23	W	8	4SU
23	W	11	C
23	W	13	C
23	W	14	A
23	W	19	G
23	W	20	U
23	W	21	A
23	W	22	G
23	W	23	A
23	W	26	A
23	W	34	G
23	W	42	C
23	W	44	G
23	W	45	U
23	W	46	7MG
23	W	47	U
23	W	48	C
23	W	49	C
23	W	61	C
23	W	63	G
23	W	64	A
23	W	68	C
23	W	70	G
23	W	73	A
23	W	74	C
23	W	75	C
23	W	76	A
24	X	3	C
24	X	9	G
24	X	18	G
24	X	19	G
24	X	20	U
24	X	21	A
24	X	31	G
24	X	42	G
24	X	47	U

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Mol	Chain	Res	Type
24	X	48	C
24	X	60	U
24	X	61	C
24	X	62	C
24	X	65	C
24	X	67	C
24	X	68	C
24	X	70	G
24	X	76	A
23	Y	2	C
23	Y	3	C
23	Y	5	G
23	Y	9	A
23	Y	13	C
23	Y	14	A
23	Y	15	G
23	Y	19	G
23	Y	20	U
23	Y	21	A
23	Y	22	G
23	Y	30	G
23	Y	31	A
23	Y	33	U
23	Y	34	G
23	Y	35	A
23	Y	39	PSU
23	Y	44	G
23	Y	45	U
23	Y	46	7MG
23	Y	47	U
23	Y	48	C
23	Y	49	C
23	Y	51	U
23	Y	53	G
23	Y	56	C
23	Y	57	G
23	Y	58	A
23	Y	62	C
23	Y	65	G
23	Y	67	C
23	Y	70	G
23	Y	73	A

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	97	G
1	A	115	G
1	A	266	G
1	A	429	U
1	A	509	A
1	A	532	A
1	A	560	U
1	A	687	A
1	A	748	C
1	A	839	U
1	A	913	A
1	A	991	U
1	A	1036	G
1	A	1065	U
1	A	1067	A
1	A	1190	G
1	A	1201	A
1	A	1285	A
1	A	1299	A
1	A	1442	G
1	A	1492	A
23	W	13	C
23	W	22	G
24	X	47	U
23	Y	44	G

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	25,23	19,21,22	1.85	5 (26%)	23,30,33	1.18	1 (4%)
23	MIA	W	37	23	29,31,32	1.88	4 (13%)	41,44,47	1.81	8 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSU	W	39	23	19,21,22	1.81	5 (26%)	23,30,33	0.96	2 (8%)
23	7MG	W	46	23	24,26,27	2.04	6 (25%)	34,39,42	2.45	10 (29%)
23	5MU	W	54	23	20,22,23	1.69	5 (25%)	25,32,35	2.07	3 (12%)
23	PSU	W	55	23	19,21,22	1.79	4 (21%)	23,30,33	1.58	2 (8%)
23	4SU	W	8	23	19,21,22	1.82	4 (21%)	23,30,33	8.03	4 (17%)
24	5MC	X	32	24	20,22,23	1.70	4 (20%)	26,32,35	1.59	4 (15%)
24	5MU	X	54	24,25	20,22,23	1.67	5 (25%)	25,32,35	1.71	4 (16%)
24	PSU	X	55	24	19,21,22	1.97	4 (21%)	23,30,33	1.04	2 (8%)
24	4SU	X	8	24	19,21,22	1.76	3 (15%)	23,30,33	37.45	2 (8%)
23	PSU	Y	32	23	19,21,22	1.86	4 (21%)	23,30,33	1.30	2 (8%)
23	MIA	Y	37	23	20,24,32	1.79	5 (25%)	27,35,47	1.82	4 (14%)
23	PSU	Y	39	23	19,21,22	1.86	6 (31%)	23,30,33	1.14	1 (4%)
23	7MG	Y	46	23	24,26,27	2.06	7 (29%)	34,39,42	2.60	10 (29%)
23	5MU	Y	54	23	20,22,23	1.80	5 (25%)	25,32,35	1.79	3 (12%)
23	PSU	Y	55	23	19,21,22	1.83	4 (21%)	23,30,33	1.06	2 (8%)
23	4SU	Y	8	23	19,21,22	1.82	4 (21%)	23,30,33	11.54	3 (13%)

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	25,23	-	0/8/25/26	0/2/2/2
23	MIA	W	37	23	-	0/16/33/34	0/3/3/3
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	24,25	-	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	-	0/6/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-7.30	1.69	1.75
23	W	46	7MG	C6-C5	5.50	1.48	1.41
23	Y	46	7MG	C6-C5	5.46	1.48	1.41
24	X	55	PSU	C5-C1'	-4.82	1.48	1.52
23	W	46	7MG	P-OP1	4.66	1.52	1.46
24	X	32	5MC	C5-C4	4.66	1.48	1.41
23	Y	37	MIA	P-OP1	4.59	1.51	1.46
23	Y	8	4SU	P-OP1	4.58	1.51	1.46
23	Y	46	7MG	P-OP1	4.52	1.51	1.46
23	W	8	4SU	P-OP1	4.50	1.51	1.46
23	Y	54	5MU	P-OP1	4.46	1.51	1.46
23	Y	55	PSU	P-OP1	4.41	1.51	1.46
24	X	8	4SU	P-OP1	4.25	1.51	1.46
23	W	55	PSU	P-OP1	4.24	1.51	1.46
23	W	37	MIA	P-OP1	4.22	1.51	1.46
23	W	39	PSU	P-OP1	4.21	1.51	1.46
24	X	32	5MC	P-OP1	4.14	1.51	1.46
23	Y	32	PSU	P-OP1	4.14	1.51	1.46
24	X	55	PSU	P-OP1	4.13	1.51	1.46
23	Y	39	PSU	P-OP1	4.12	1.51	1.46
23	W	32	PSU	P-OP1	4.11	1.51	1.46
23	Y	32	PSU	C5-C1'	-4.06	1.48	1.52
24	X	8	4SU	O2-C2	4.03	1.27	1.21
23	Y	55	PSU	C5-C1'	-4.00	1.48	1.52
24	X	54	5MU	P-OP1	4.00	1.51	1.46
23	W	54	5MU	P-OP1	3.96	1.51	1.46
23	W	39	PSU	C5-C1'	-3.78	1.48	1.52
23	Y	8	4SU	O2-C2	3.79	1.26	1.21
23	W	32	PSU	C5-C1'	-3.72	1.49	1.52
23	W	55	PSU	C5-C1'	-3.71	1.49	1.52
23	W	8	4SU	O2-C2	3.70	1.26	1.21
23	Y	54	5MU	O2-C2	3.63	1.26	1.21
23	W	8	4SU	C4-S4	-3.63	1.60	1.67
23	W	32	PSU	C4-C5	3.56	1.49	1.40
23	Y	32	PSU	C4-C5	3.53	1.49	1.40
23	Y	37	MIA	C5-C4	3.51	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	54	5MU	C2-N1	3.49	1.42	1.38
24	X	8	4SU	C4-S4	-3.45	1.60	1.67
23	Y	54	5MU	C2-N1	3.45	1.42	1.38
23	Y	54	5MU	C4-C5	3.45	1.48	1.40
23	Y	39	PSU	C5-C1'	-3.42	1.49	1.52
23	W	8	4SU	C2-N1	3.41	1.42	1.38
24	X	54	5MU	C4-C5	3.38	1.48	1.40
23	Y	8	4SU	C4-S4	-3.37	1.60	1.67
23	W	54	5MU	C4-C5	3.37	1.48	1.40
23	Y	8	4SU	C2-N1	3.36	1.42	1.38
23	W	55	PSU	C4-C5	3.31	1.48	1.40
23	Y	37	MIA	C6-N6	3.30	1.35	1.28
23	Y	39	PSU	O2-C2	3.28	1.26	1.21
23	W	39	PSU	C4-C5	3.27	1.48	1.40
23	Y	55	PSU	O2-C2	3.26	1.26	1.21
24	X	55	PSU	C4-C5	3.25	1.48	1.40
23	Y	39	PSU	C4-C5	3.21	1.48	1.40
23	W	32	PSU	O2-C2	3.18	1.25	1.21
24	X	55	PSU	O2-C2	3.14	1.25	1.21
24	X	54	5MU	C2-N1	3.06	1.41	1.38
23	Y	32	PSU	O2-C2	3.05	1.25	1.21
23	W	54	5MU	O2-C2	3.04	1.25	1.21
23	W	37	MIA	C5-C4	3.02	1.47	1.40
23	W	46	7MG	C2-N3	3.00	1.37	1.33
23	Y	46	7MG	C2-N3	2.99	1.37	1.33
23	Y	46	7MG	C5-C4	2.98	1.49	1.39
24	X	54	5MU	O2-C2	2.95	1.25	1.21
23	Y	55	PSU	C4-C5	2.93	1.47	1.40
23	W	46	7MG	C5-N7	-2.88	1.34	1.39
23	W	55	PSU	O2-C2	2.86	1.25	1.21
23	Y	46	7MG	C5-N7	-2.76	1.34	1.39
23	W	46	7MG	C2-N2	2.70	1.36	1.32
23	W	46	7MG	C5-C4	2.69	1.48	1.39
23	W	39	PSU	O2-C2	2.69	1.25	1.21
23	Y	46	7MG	C2-N2	2.68	1.36	1.32
24	X	32	5MC	C2-N1	2.64	1.41	1.38
23	W	37	MIA	C4-N9	-2.57	1.34	1.37
23	Y	37	MIA	C6-C5	2.52	1.49	1.44
24	X	32	5MC	O2-C2	2.50	1.25	1.21
23	Y	39	PSU	O4'-C1'	-2.36	1.40	1.44
23	Y	37	MIA	C4-N9	-2.30	1.34	1.37
23	W	54	5MU	C4-N3	-2.25	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	46	7MG	CM7-N7	2.22	1.49	1.46
24	X	54	5MU	C4-N3	-2.18	1.33	1.36
23	W	32	PSU	C4-N3	-2.15	1.33	1.36
23	Y	54	5MU	C4-N3	-2.13	1.33	1.36
23	Y	39	PSU	O5'-C5'	-2.09	1.41	1.44
23	W	39	PSU	O5'-C5'	-2.03	1.41	1.44

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	8	4SU	C4-N3-C2	179.47	129.28	121.60
23	Y	8	4SU	C4-N3-C2	54.70	123.94	121.60
23	W	8	4SU	C4-N3-C2	37.68	123.21	121.60
23	Y	46	7MG	N3-C4-N9	7.78	139.09	126.80
23	W	46	7MG	N3-C4-N9	7.69	138.96	126.80
23	Y	46	7MG	C6-N1-C2	7.62	124.50	120.20
23	Y	8	4SU	C2-N1-C1'	7.62	122.98	118.21
23	W	54	5MU	C6-N1-C2	-7.44	120.29	122.41
23	W	8	4SU	C2-N1-C1'	6.84	122.50	118.21
23	W	37	MIA	C5-C4-N3	-6.07	119.08	126.07
23	Y	37	MIA	C5-C4-N3	-6.07	119.08	126.07
24	X	54	5MU	N3-C2-N1	5.87	120.88	115.97
24	X	8	4SU	C2-N1-C1'	5.86	121.88	118.21
23	W	55	PSU	C5-C1'-C2'	-5.85	104.87	115.73
23	W	46	7MG	C6-N1-C2	5.69	123.41	120.20
23	Y	54	5MU	C6-N1-C2	-5.45	120.86	122.41
23	W	37	MIA	N3-C4-N9	5.45	134.91	126.91
23	W	46	7MG	N7-C8-N9	-5.43	95.92	103.13
23	Y	37	MIA	N3-C4-N9	5.37	134.78	126.91
23	W	54	5MU	N3-C2-N1	5.32	120.41	115.97
23	W	46	7MG	C5-C4-N3	-4.91	118.01	126.61
23	Y	46	7MG	C5-C4-N3	-4.89	118.04	126.61
23	Y	46	7MG	N7-C8-N9	-4.84	96.71	103.13
23	Y	54	5MU	C2-N1-C1'	4.68	121.14	118.21
23	Y	32	PSU	C5-C1'-C2'	-4.66	107.09	115.73
24	X	32	5MC	C2-N3-C4	4.40	119.71	115.50
23	W	32	PSU	C5-C1'-C2'	-4.28	107.79	115.73
23	Y	54	5MU	N3-C2-N1	4.22	119.49	115.97
23	W	37	MIA	C2-N3-C4	3.91	120.73	115.22
24	X	54	5MU	C6-N1-C2	-3.87	121.31	122.41
23	Y	39	PSU	O4'-C1'-C5	-3.85	103.34	109.80
24	X	32	5MC	C6-N1-C2	3.52	121.38	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	46	7MG	C8-N9-C1'	-3.51	111.36	121.06
23	W	46	7MG	C8-N7-C5	3.50	115.81	108.83
23	W	37	MIA	N6-C6-N1	3.46	122.75	118.63
24	X	32	5MC	C5-C6-N1	-3.36	119.00	122.02
23	Y	46	7MG	C8-N7-C5	3.26	115.33	108.83
23	W	46	7MG	C8-N9-C1'	-3.22	112.17	121.06
23	W	54	5MU	C2-N1-C1'	3.19	120.21	118.21
24	X	54	5MU	C5-C6-N1	-3.14	119.20	122.02
24	X	55	PSU	C5-C1'-C2'	-3.05	110.08	115.73
23	W	37	MIA	C2-N1-C6	3.04	122.32	113.31
23	Y	8	4SU	N3-C2-N1	2.97	118.45	115.97
23	W	37	MIA	C5-C6-N1	-2.88	117.40	120.46
24	X	32	5MC	N4-C4-N3	2.87	121.09	116.99
23	Y	46	7MG	C6-C5-C4	2.87	119.92	116.01
23	W	46	7MG	C6-C5-C4	2.84	119.87	116.01
23	W	8	4SU	N3-C2-N1	2.71	118.24	115.97
23	Y	37	MIA	C4-C5-N7	-2.61	106.89	109.41
23	Y	37	MIA	C5-C6-N1	-2.54	117.89	120.10
23	Y	32	PSU	C4-N3-C2	-2.38	120.53	125.36
23	Y	55	PSU	C4-N3-C2	-2.37	120.56	125.36
23	W	46	7MG	C8-N9-C4	2.35	118.11	110.66
23	W	39	PSU	C5-C1'-C2'	-2.35	111.37	115.73
23	W	37	MIA	C4-C5-N7	-2.32	107.17	109.41
23	W	39	PSU	C4-N3-C2	-2.31	120.68	125.36
23	Y	46	7MG	CM7-N7-C5	2.29	131.81	123.46
23	W	55	PSU	C4-N3-C2	-2.24	120.82	125.36
23	W	37	MIA	N3-C2-N1	-2.22	122.87	126.87
23	Y	46	7MG	C8-N9-C4	2.20	117.62	110.66
24	X	54	5MU	C4-N3-C2	-2.19	120.89	125.39
24	X	55	PSU	C4-N3-C2	-2.18	120.93	125.36
23	W	46	7MG	CM7-N7-C5	2.15	131.30	123.46
23	Y	46	7MG	C5-C4-N9	-2.15	102.86	106.08
23	Y	55	PSU	O4'-C1'-C2'	2.11	108.03	104.43
23	W	8	4SU	C5-C4-N3	2.09	119.65	116.04
23	W	46	7MG	C5-C4-N9	-2.04	103.03	106.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 264 ligands modelled in this entry, 262 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	PCY	A	3231	-	42,42,42	1.62	6 (14%)	65,65,65	1.76	13 (20%)
27	SF4	D	501	4	12,12,12	22.91	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	PCY	A	3231	-	-	0/33/67/67	0/3/3/3
27	SF4	D	501	4	-	0/0/48/48	0/6/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	501	SF4	S3-FE2	-24.24	2.16	2.33
27	D	501	SF4	S4-FE2	-23.51	2.17	2.33
27	D	501	SF4	S1-FE3	-23.49	2.17	2.33
27	D	501	SF4	S1-FE2	-23.30	2.17	2.33
27	D	501	SF4	S2-FE1	-23.16	2.17	2.33
27	D	501	SF4	S4-FE3	-23.13	2.17	2.33
27	D	501	SF4	S3-FE1	-23.02	2.17	2.33
27	D	501	SF4	S1-FE4	-22.99	2.17	2.33
27	D	501	SF4	S4-FE1	-22.50	2.18	2.33
27	D	501	SF4	S2-FE3	-22.36	2.18	2.33
27	D	501	SF4	S2-FE4	-21.83	2.18	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	501	SF4	S3-FE4	-21.26	2.19	2.33
26	A	3231	PCY	C28-C32	-5.36	1.39	1.49
26	A	3231	PCY	C34-C30	-5.31	1.40	1.51
26	A	3231	PCY	C27-C23	-3.62	1.40	1.50
26	A	3231	PCY	C3-C6	2.97	1.57	1.52
26	A	3231	PCY	C22-N20	-2.71	1.34	1.39
26	A	3231	PCY	C17-N20	2.16	1.48	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	3231	PCY	C6-C3-N2	7.74	114.08	107.39
26	A	3231	PCY	C7-C3-C8	-4.43	94.46	102.92
26	A	3231	PCY	C18-O21-C23	-4.38	107.00	116.57
26	A	3231	PCY	C8-C17-N20	-2.95	107.50	112.80
26	A	3231	PCY	O21-C23-C27	2.91	119.12	112.32
26	A	3231	PCY	C6-C3-C8	2.65	114.66	111.33
26	A	3231	PCY	C13-C7-C15	-2.52	109.98	115.01
26	A	3231	PCY	O21-C18-C15	2.43	112.92	108.01
26	A	3231	PCY	C10-N4-C9	2.20	122.22	115.70
26	A	3231	PCY	O36-C31-C27	-2.16	116.91	121.11
26	A	3231	PCY	C34-C30-C35	-2.09	116.08	120.33
26	A	3231	PCY	C30-C27-C23	2.07	126.64	120.41
26	A	3231	PCY	C34-C30-C27	2.08	124.53	121.80

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.