



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:47 PM BST

PDB ID : 3J5Y
EMDB ID: : EMD-5801
Title : Structure of the mammalian ribosomal pre-termination complex associated with eRF1-eRF3-GDPNP
Authors : des Georges, A.; Hashem, Y.; Unbehaun, A.; Grassucci, R.A.; Taylor, D.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.
Deposited on : 2013-11-21
Resolution : 9.70 Å(reported)
Based on PDB ID : 2KTU, 1R5O, 3E1Y, 1R5B, 3VMF

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

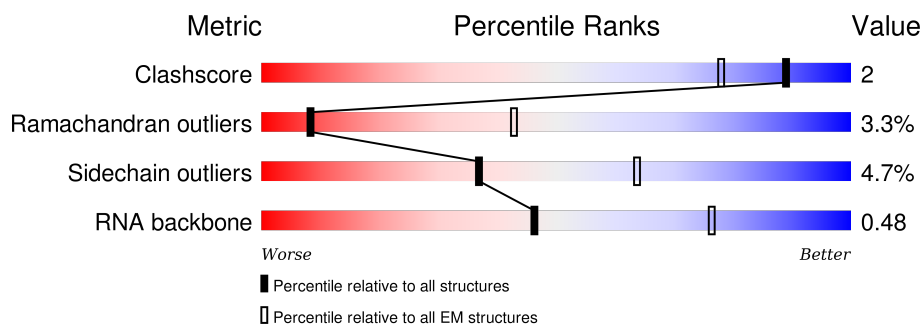
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	414	70% 25% 5%
2	B	428	70% 25% .
3	C	10	60% 40%
4	D	88	38% 34% 28%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8724 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	414	Total	C	N	O	S	0	0
			3269	2080	557	621	11		

- Molecule 2 is a protein called Eukaryotic peptide chain release factor GTP-binding subunit ERF3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	428	Total	C	N	O	S	0	0
			3367	2144	578	624	21		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	369	ILE	ASN	CONFLICT	UNP P15170
B	389	SER	ASN	CONFLICT	UNP P15170
B	407	ILE	LEU	CONFLICT	UNP P15170
B	418	THR	ILE	CONFLICT	UNP P15170
B	436	ILE	VAL	CONFLICT	UNP P15170

- Molecule 3 is a RNA chain called 5'-R(*AP*UP*UP*GP*UP*AP*AP*AP*AP*A)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	10	Total	C	N	O	P	0	0
			212	97	41	65	9		

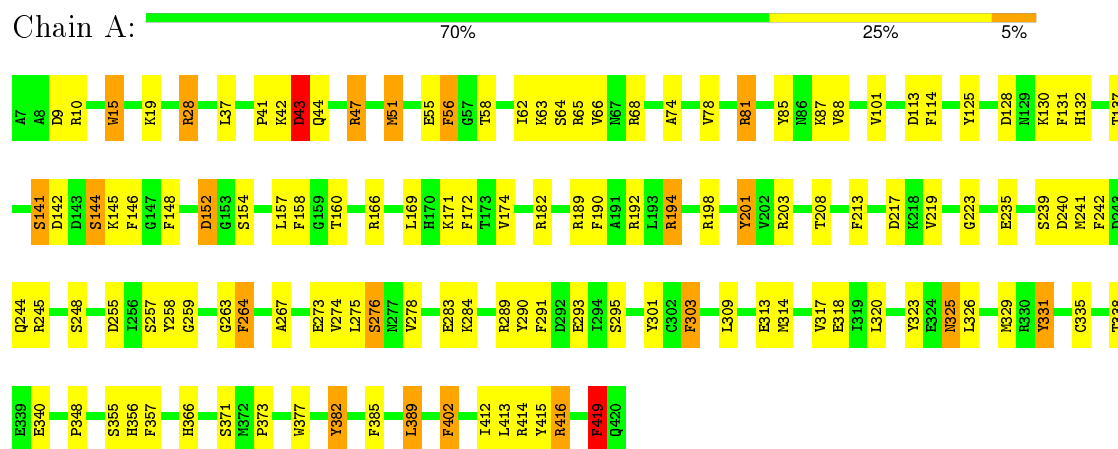
- Molecule 4 is a RNA chain called tRNA-Leu.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	88	Total	C	N	O	P	0	0
			1876	836	339	614	87		

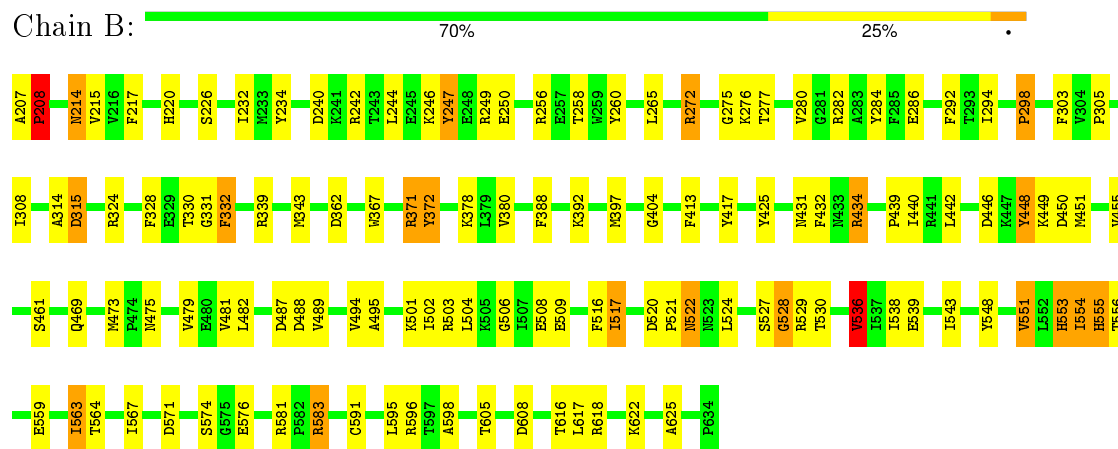
3 Residue-property plots

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Eukaryotic peptide chain release factor subunit 1



- Molecule 2: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A



- Molecule 3: 5'-R(*AP*UP*UP*GP*UP*AP*AP*AP*AP*A)-3'



- Molecule 4: tRNA-Leu

Response	Percentage
Yes, more action is needed	38%
No, the U.S. is doing enough	34%
Don't know	28%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	48973	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each Particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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 >2	RMSZ	# Z >2
1	A	1.62	28/3322 (0.8%)	2.00	87/4466 (1.9%)
2	B	1.57	14/3434 (0.4%)	1.98	91/4630 (2.0%)
3	C	3.46	38/238 (16.0%)	3.23	39/369 (10.6%)
4	D	3.24	252/2095 (12.0%)	3.32	394/3266 (12.1%)
All	All	2.15	332/9089 (3.7%)	2.44	611/12731 (4.8%)

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
1	A	0	17
2	B	0	23
3	C	0	7
4	D	0	42
All	All	0	89

All (332) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	14	A	P-O5'	-13.49	1.46	1.59
4	D	77	G	N3-C4	-12.40	1.26	1.35
4	D	17	C	N1-C6	12.07	1.44	1.37
4	D	6	G	C6-N1	11.74	1.47	1.39
4	D	22	C	P-O5'	-11.66	1.48	1.59
4	D	20	G	N7-C5	-11.39	1.32	1.39
4	D	39	A	N9-C4	-11.27	1.31	1.37
4	D	85	A	N9-C4	11.16	1.44	1.37
3	C	99	A	C3'-C2'	11.09	1.65	1.52
4	D	80	C	N3-C4	10.79	1.41	1.33
4	D	22	C	O3'-P	-10.73	1.48	1.61
3	C	93	G	N3-C4	-10.54	1.28	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	31	G	P-O5'	-10.53	1.49	1.59
4	D	56	G	C2-N3	10.41	1.41	1.32
4	D	40	G	N7-C5	10.40	1.45	1.39
4	D	29	G	C2-N3	10.38	1.41	1.32
3	C	93	G	C6-N1	10.35	1.46	1.39
4	D	5	G	N3-C4	10.35	1.42	1.35
4	D	78	C	C2-N3	10.34	1.44	1.35
4	D	60	C	P-O5'	-10.30	1.49	1.59
3	C	95	A	C2'-C1'	-10.25	1.42	1.53
4	D	83	G	N9-C8	-10.12	1.30	1.37
4	D	86	C	N3-C4	10.12	1.41	1.33
4	D	76	C	N3-C4	10.03	1.41	1.33
4	D	34	A	N3-C4	10.01	1.40	1.34
4	D	13	G	C5-C4	-9.94	1.31	1.38
4	D	31	G	C6-N1	9.83	1.46	1.39
4	D	38	A	N3-C4	-9.72	1.29	1.34
4	D	78	C	N1-C6	9.72	1.43	1.37
4	D	15	G	P-O5'	-9.53	1.50	1.59
4	D	53	A	N3-C4	9.46	1.40	1.34
4	D	86	C	N1-C6	9.43	1.42	1.37
4	D	45	C	P-O5'	-9.26	1.50	1.59
4	D	22	C	C4-C5	9.22	1.50	1.43
4	D	84	C	N1-C2	-9.00	1.31	1.40
4	D	29	G	C8-N7	-8.86	1.25	1.30
4	D	87	C	P-O5'	8.86	1.68	1.59
4	D	5	G	N9-C4	-8.82	1.30	1.38
4	D	82	C	C2'-C1'	-8.77	1.43	1.53
4	D	32	G	P-O5'	-8.62	1.51	1.59
4	D	71	A	N9-C8	8.62	1.44	1.37
4	D	1	G	C8-N7	-8.61	1.25	1.30
4	D	18	U	C4'-C3'	8.54	1.62	1.53
4	D	67	U	C2-N3	8.49	1.43	1.37
4	D	57	G	C2-N3	-8.46	1.25	1.32
4	D	63	G	P-O5'	-8.43	1.51	1.59
4	D	19	G	P-O5'	-8.39	1.51	1.59
4	D	21	U	N1-C6	8.38	1.45	1.38
4	D	11	C	N1-C6	-8.36	1.32	1.37
4	D	46	C	N1-C6	-8.34	1.32	1.37
3	C	90	A	N9-C4	8.31	1.42	1.37
4	D	55	G	N3-C4	8.29	1.41	1.35
4	D	84	C	N1-C6	8.28	1.42	1.37
4	D	80	C	N1-C6	-8.20	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	68	C	N1-C6	8.17	1.42	1.37
4	D	9	U	C5'-C4'	8.15	1.61	1.51
4	D	69	G	C2-N2	-8.15	1.26	1.34
4	D	25	A	N3-C4	-8.08	1.30	1.34
4	D	3	G	C6-N1	-7.89	1.34	1.39
3	C	91	U	O3'-P	-7.83	1.51	1.61
4	D	33	G	C8-N7	7.80	1.35	1.30
4	D	4	G	N3-C4	-7.73	1.30	1.35
4	D	61	C	O3'-P	-7.72	1.51	1.61
4	D	62	G	C2'-C1'	-7.68	1.45	1.53
4	D	79	C	C2'-C1'	-7.64	1.45	1.53
4	D	46	C	N3-C4	7.59	1.39	1.33
4	D	54	G	C8-N7	-7.56	1.26	1.30
4	D	51	G	C4'-C3'	7.56	1.61	1.53
4	D	7	G	C5'-C4'	7.54	1.60	1.51
4	D	29	G	C5-C4	7.53	1.43	1.38
4	D	42	U	C2-N3	7.50	1.43	1.37
3	C	99	A	P-O5'	-7.49	1.52	1.59
4	D	10	G	N3-C4	7.48	1.40	1.35
4	D	50	C	P-O5'	-7.44	1.52	1.59
4	D	25	A	N9-C8	7.35	1.43	1.37
4	D	29	G	N9-C4	7.33	1.43	1.38
4	D	19	G	N7-C5	-7.33	1.34	1.39
4	D	66	U	O3'-P	-7.30	1.52	1.61
4	D	17	C	C4'-C3'	7.28	1.61	1.53
3	C	90	A	N3-C4	7.26	1.39	1.34
3	C	91	U	C4'-O4'	-7.26	1.36	1.45
4	D	10	G	C8-N7	-7.23	1.26	1.30
4	D	15	G	N7-C5	-7.15	1.34	1.39
3	C	90	A	C6-N1	7.14	1.40	1.35
3	C	95	A	N9-C4	7.13	1.42	1.37
4	D	15	G	C5'-C4'	7.10	1.59	1.51
4	D	35	C	C4'-C3'	-7.09	1.45	1.53
4	D	6	G	P-O5'	7.06	1.66	1.59
4	D	44	C	P-O5'	-7.06	1.52	1.59
4	D	22	C	C3'-O3'	7.05	1.52	1.42
3	C	95	A	N7-C5	7.01	1.43	1.39
3	C	90	A	O4'-C1'	-7.00	1.32	1.41
3	C	95	A	N3-C4	6.96	1.39	1.34
4	D	64	G	C2-N2	-6.93	1.27	1.34
4	D	83	G	N1-C2	-6.93	1.32	1.37
4	D	28	C	N3-C4	6.92	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	591	CYS	CB-SG	6.92	1.94	1.82
4	D	10	G	C6-N1	-6.91	1.34	1.39
2	B	404	GLY	N-CA	-6.91	1.35	1.46
4	D	77	G	C4'-C3'	6.90	1.60	1.53
4	D	75	C	C4-N4	-6.88	1.27	1.33
4	D	53	A	C6-N1	6.85	1.40	1.35
4	D	17	C	N3-C4	6.80	1.38	1.33
4	D	1	G	N7-C5	6.80	1.43	1.39
4	D	57	G	O3'-P	-6.80	1.52	1.61
3	C	97	A	C8-N7	-6.78	1.26	1.31
2	B	559	GLU	CD-OE2	6.77	1.33	1.25
4	D	14	A	N7-C5	6.76	1.43	1.39
4	D	5	G	C4'-C3'	6.75	1.60	1.53
4	D	6	G	C8-N7	-6.73	1.26	1.30
4	D	61	C	N1-C6	6.72	1.41	1.37
4	D	55	G	N7-C5	6.71	1.43	1.39
4	D	50	C	C5'-C4'	6.70	1.59	1.51
3	C	91	U	C2-N3	6.68	1.42	1.37
4	D	37	C	C3'-O3'	6.67	1.51	1.42
4	D	24	A	C5-C4	-6.64	1.34	1.38
4	D	38	A	C3'-C2'	6.63	1.60	1.52
4	D	62	G	C2-N2	-6.62	1.27	1.34
4	D	3	G	C2-N3	6.60	1.38	1.32
4	D	31	G	N7-C5	-6.60	1.35	1.39
4	D	81	C	C3'-C2'	6.60	1.60	1.52
1	A	248	SER	CA-CB	6.59	1.62	1.52
4	D	64	G	C6-N1	-6.56	1.34	1.39
4	D	64	G	C8-N7	6.55	1.34	1.30
4	D	21	U	C2-N3	-6.51	1.33	1.37
4	D	75	C	C3'-O3'	6.51	1.51	1.42
4	D	62	G	P-O5'	-6.50	1.53	1.59
4	D	20	G	N3-C4	6.48	1.40	1.35
4	D	37	C	C4'-C3'	-6.47	1.46	1.53
4	D	62	G	N9-C8	6.46	1.42	1.37
4	D	81	C	C2-N3	6.40	1.40	1.35
4	D	31	G	N3-C4	6.38	1.40	1.35
4	D	56	G	N7-C5	6.38	1.43	1.39
4	D	78	C	C5'-C4'	6.38	1.59	1.51
4	D	39	A	N7-C5	-6.33	1.35	1.39
4	D	72	U	O4'-C1'	-6.33	1.33	1.41
4	D	20	G	N9-C4	6.33	1.43	1.38
4	D	74	C	C4-C5	6.32	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	62	G	N9-C4	-6.32	1.32	1.38
4	D	84	C	N3-C4	6.31	1.38	1.33
4	D	2	C	O4'-C1'	-6.30	1.33	1.41
4	D	79	C	N3-C4	6.30	1.38	1.33
4	D	31	G	C8-N7	6.30	1.34	1.30
4	D	12	C	N3-C4	6.29	1.38	1.33
3	C	93	G	O3'-P	-6.28	1.53	1.61
4	D	10	G	N9-C4	-6.28	1.32	1.38
4	D	88	A	P-O5'	-6.28	1.53	1.59
4	D	62	G	C5-C4	-6.27	1.33	1.38
4	D	66	U	C4-O4	-6.26	1.18	1.23
2	B	527	SER	CA-CB	6.26	1.62	1.52
4	D	35	C	C4-C5	6.25	1.48	1.43
4	D	71	A	C3'-C2'	-6.25	1.45	1.52
4	D	6	G	N7-C5	6.23	1.43	1.39
4	D	23	A	O3'-P	-6.23	1.53	1.61
4	D	77	G	C5'-C4'	6.22	1.58	1.51
1	A	125	TYR	CA-CB	6.21	1.67	1.53
4	D	76	C	C2-N3	6.20	1.40	1.35
4	D	44	C	O3'-P	-6.19	1.53	1.61
4	D	19	G	O3'-P	-6.19	1.53	1.61
3	C	99	A	C6-N6	-6.18	1.29	1.33
1	A	154	SER	CB-OG	6.16	1.50	1.42
4	D	65	G	C8-N7	6.16	1.34	1.30
2	B	260	TYR	CG-CD2	6.16	1.47	1.39
1	A	235	GLU	CG-CD	-6.15	1.42	1.51
4	D	80	C	C4'-C3'	6.12	1.59	1.53
4	D	36	U	C5'-C4'	6.12	1.58	1.51
4	D	80	C	C5'-C4'	6.12	1.58	1.51
4	D	3	G	N3-C4	-6.11	1.31	1.35
4	D	72	U	C5'-C4'	6.09	1.58	1.51
4	D	82	C	P-O5'	-6.07	1.53	1.59
4	D	31	G	C5-C6	6.05	1.48	1.42
4	D	36	U	C3'-O3'	6.04	1.50	1.42
3	C	96	A	C5'-C4'	6.04	1.58	1.51
1	A	192	ARG	CD-NE	6.03	1.56	1.46
3	C	97	A	N3-C4	-6.03	1.31	1.34
4	D	29	G	C5'-C4'	6.02	1.58	1.51
4	D	86	C	O3'-P	-6.00	1.53	1.61
4	D	65	G	O4'-C1'	5.98	1.49	1.41
4	D	8	U	C2-N3	5.97	1.42	1.37
4	D	47	U	P-O5'	-5.96	1.53	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	90	A	C5-C6	-5.94	1.35	1.41
4	D	62	G	C4'-C3'	5.93	1.59	1.53
3	C	92	U	C4'-C3'	5.91	1.59	1.53
3	C	92	U	O3'-P	-5.90	1.54	1.61
1	A	313	GLU	CA-CB	5.90	1.67	1.53
4	D	41	A	C5-C4	5.90	1.42	1.38
3	C	99	A	C5'-C4'	5.89	1.58	1.51
4	D	3	G	P-O5'	5.88	1.65	1.59
1	A	263	GLY	CA-C	5.88	1.61	1.51
4	D	30	G	C5-C6	-5.88	1.36	1.42
4	D	19	G	C8-N7	5.86	1.34	1.30
4	D	6	G	C5'-C4'	5.86	1.58	1.51
4	D	11	C	N3-C4	5.85	1.38	1.33
4	D	41	A	N9-C4	5.83	1.41	1.37
3	C	90	A	C5'-C4'	5.83	1.58	1.51
3	C	99	A	C4'-O4'	5.82	1.53	1.45
4	D	24	A	C2-N3	-5.81	1.28	1.33
4	D	59	U	C4'-C3'	5.81	1.59	1.53
4	D	86	C	C5'-C4'	5.81	1.58	1.51
4	D	60	C	C2'-C1'	-5.81	1.47	1.53
4	D	46	C	P-O5'	-5.80	1.53	1.59
3	C	96	A	C4'-C3'	5.79	1.59	1.53
4	D	70	A	C2'-C1'	-5.79	1.47	1.53
4	D	37	C	C4-C5	5.78	1.47	1.43
4	D	2	C	N3-C4	5.77	1.38	1.33
4	D	11	C	O3'-P	-5.77	1.54	1.61
3	C	99	A	C6-N1	5.75	1.39	1.35
2	B	528	GLY	CA-C	-5.75	1.42	1.51
4	D	35	C	C2-N3	-5.71	1.31	1.35
4	D	26	G	C5'-C4'	5.71	1.58	1.51
4	D	15	G	C6-N1	5.69	1.43	1.39
1	A	148	PHE	CG-CD2	5.69	1.47	1.38
4	D	27	G	C1'-N9	5.69	1.57	1.48
4	D	85	A	C3'-O3'	5.68	1.50	1.42
4	D	19	G	C5-C4	-5.68	1.34	1.38
4	D	59	U	C2-O2	5.67	1.27	1.22
3	C	95	A	C6-N1	5.67	1.39	1.35
4	D	2	C	C3'-C2'	-5.66	1.46	1.52
4	D	74	C	P-O5'	-5.66	1.54	1.59
4	D	45	C	C4-N4	-5.65	1.28	1.33
4	D	48	C	N1-C6	5.64	1.40	1.37
4	D	33	G	C2-N2	-5.64	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	339	ARG	CD-NE	5.64	1.56	1.46
4	D	62	G	O3'-P	-5.64	1.54	1.61
2	B	286	GLU	CB-CG	5.61	1.62	1.52
4	D	65	G	N1-C2	5.61	1.42	1.37
4	D	4	G	N9-C8	5.60	1.41	1.37
3	C	98	A	O3'-P	-5.60	1.54	1.61
4	D	1	G	N3-C4	-5.59	1.31	1.35
4	D	61	C	C4-C5	-5.58	1.38	1.43
4	D	27	G	N9-C8	-5.58	1.33	1.37
2	B	417	TYR	CG-CD2	5.56	1.46	1.39
4	D	23	A	C4'-C3'	5.56	1.59	1.53
4	D	23	A	C6-N1	-5.54	1.31	1.35
4	D	24	A	C5-C6	-5.53	1.36	1.41
1	A	15	TRP	CB-CG	5.52	1.60	1.50
1	A	366	HIS	N-CA	5.50	1.57	1.46
4	D	20	G	C8-N7	5.49	1.34	1.30
4	D	85	A	C2'-C1'	-5.49	1.47	1.53
1	A	87	LYS	CA-CB	5.48	1.66	1.53
4	D	33	G	C5-C4	-5.46	1.34	1.38
4	D	50	C	C4-N4	-5.46	1.29	1.33
4	D	52	U	C2-N3	5.46	1.41	1.37
4	D	75	C	O4'-C1'	5.46	1.48	1.41
4	D	70	A	C5-C6	5.46	1.46	1.41
4	D	33	G	N7-C5	5.45	1.42	1.39
2	B	234	TYR	CG-CD2	5.44	1.46	1.39
4	D	24	A	C1'-N9	-5.44	1.39	1.46
1	A	318	GLU	CB-CG	5.42	1.62	1.52
4	D	74	C	C2'-C1'	-5.41	1.47	1.53
4	D	82	C	O4'-C1'	5.39	1.48	1.41
4	D	63	G	C6-N1	-5.39	1.35	1.39
1	A	213	PHE	CB-CG	-5.38	1.42	1.51
4	D	3	G	C8-N7	-5.38	1.27	1.30
4	D	7	G	C3'-O3'	5.38	1.49	1.42
4	D	56	G	C1'-N9	5.37	1.56	1.48
4	D	22	C	N3-C4	5.36	1.37	1.33
4	D	54	G	C2-N3	-5.36	1.28	1.32
1	A	28	ARG	NE-CZ	5.36	1.40	1.33
4	D	4	G	C2-N3	-5.35	1.28	1.32
3	C	95	A	C4'-O4'	-5.33	1.38	1.45
4	D	33	G	O3'-P	-5.32	1.54	1.61
4	D	17	C	P-O5'	-5.32	1.54	1.59
4	D	61	C	C2-N3	-5.32	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	93	G	N9-C8	5.32	1.41	1.37
2	B	548	TYR	CZ-OH	5.31	1.46	1.37
1	A	235	GLU	CB-CG	5.30	1.62	1.52
3	C	97	A	C5-C4	5.30	1.42	1.38
4	D	47	U	C5'-C4'	5.30	1.57	1.51
1	A	419	PHE	CG-CD1	5.29	1.46	1.38
1	A	295	SER	CA-CB	5.29	1.60	1.52
4	D	2	C	C4-N4	-5.28	1.29	1.33
4	D	16	C	C3'-O3'	-5.28	1.34	1.42
4	D	38	A	P-O5'	-5.26	1.54	1.59
4	D	80	C	C2'-C1'	-5.26	1.47	1.53
4	D	51	G	N3-C4	-5.25	1.31	1.35
1	A	273	GLU	CD-OE2	5.25	1.31	1.25
4	D	1	G	C2'-C1'	5.25	1.59	1.53
4	D	16	C	C5'-C4'	5.25	1.57	1.51
4	D	24	A	N9-C8	5.24	1.42	1.37
4	D	34	A	C4'-C3'	5.24	1.58	1.53
4	D	88	A	C3'-C2'	5.23	1.58	1.52
4	D	32	G	C2-N2	-5.22	1.29	1.34
4	D	63	G	C2-N2	5.22	1.39	1.34
3	C	90	A	C5-C4	-5.21	1.35	1.38
4	D	42	U	P-O5'	-5.21	1.54	1.59
4	D	73	C	C5'-C4'	5.20	1.57	1.51
4	D	83	G	N7-C5	-5.19	1.36	1.39
4	D	10	G	C5'-C4'	5.18	1.57	1.51
1	A	258	TYR	CB-CG	-5.17	1.43	1.51
4	D	39	A	C6-N6	5.17	1.38	1.33
1	A	55	GLU	CG-CD	5.16	1.59	1.51
4	D	68	C	C5-C6	5.16	1.38	1.34
1	A	371	SER	CA-CB	5.16	1.60	1.52
1	A	125	TYR	CB-CG	5.16	1.59	1.51
2	B	508	GLU	N-CA	-5.16	1.36	1.46
3	C	90	A	O3'-P	-5.15	1.54	1.61
1	A	223	GLY	CA-C	-5.15	1.43	1.51
4	D	3	G	C2'-C1'	-5.15	1.47	1.53
4	D	32	G	O4'-C1'	5.15	1.48	1.41
1	A	415	TYR	CD1-CE1	5.14	1.47	1.39
4	D	3	G	C5'-C4'	5.14	1.57	1.51
3	C	97	A	N7-C5	5.13	1.42	1.39
4	D	40	G	C3'-O3'	5.12	1.49	1.42
4	D	31	G	C5-C4	-5.12	1.34	1.38
4	D	87	C	O3'-P	-5.11	1.55	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	40	G	C4'-C3'	-5.11	1.47	1.52
4	D	80	C	O4'-C1'	5.11	1.48	1.41
4	D	74	C	N1-C2	-5.11	1.35	1.40
3	C	90	A	C8-N7	5.10	1.35	1.31
1	A	44	GLN	CG-CD	5.10	1.62	1.51
4	D	85	A	O4'-C1'	5.10	1.48	1.41
4	D	13	G	O3'-P	-5.09	1.55	1.61
4	D	5	G	C5'-C4'	5.09	1.57	1.51
4	D	15	G	O3'-P	-5.09	1.55	1.61
1	A	9	ASP	CA-CB	5.09	1.65	1.53
4	D	34	A	N1-C2	-5.08	1.29	1.34
2	B	284	TYR	CB-CG	-5.06	1.44	1.51
4	D	72	U	C1'-N1	5.06	1.56	1.48
4	D	58	U	C2-N3	-5.06	1.34	1.37
1	A	189	ARG	CD-NE	5.05	1.55	1.46
4	D	4	G	C5-C4	5.05	1.41	1.38
3	C	96	A	P-O5'	-5.04	1.54	1.59
2	B	450	ASP	CA-CB	5.04	1.65	1.53
4	D	53	A	N1-C2	-5.04	1.29	1.34
4	D	85	A	C8-N7	-5.04	1.28	1.31
1	A	293	GLU	CB-CG	5.03	1.61	1.52
4	D	45	C	C5'-C4'	5.03	1.57	1.51
4	D	44	C	N1-C2	5.02	1.45	1.40
4	D	36	U	C5-C6	5.01	1.38	1.34
4	D	69	G	C3'-C2'	-5.01	1.47	1.52
4	D	64	G	O5'-C5'	5.00	1.52	1.44

All (611) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	91	U	P-O3'-C3'	20.04	143.75	119.70
4	D	23	A	P-O3'-C3'	19.36	142.93	119.70
1	A	203	ARG	NE-CZ-NH2	-17.01	111.80	120.30
4	D	13	G	N1-C6-O6	16.61	129.87	119.90
4	D	80	C	N3-C4-C5	-15.23	115.81	121.90
4	D	64	G	C5-C6-O6	-15.16	119.50	128.60
4	D	37	C	C6-N1-C2	-14.99	114.30	120.30
2	B	242	ARG	NE-CZ-NH1	14.57	127.58	120.30
1	A	166	ARG	NE-CZ-NH2	14.52	127.56	120.30
2	B	282	ARG	NE-CZ-NH2	-14.47	113.06	120.30
1	A	303	PHE	CB-CG-CD1	13.80	130.46	120.80
1	A	416	ARG	NE-CZ-NH1	13.72	127.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	50	C	O4'-C1'-N1	13.71	119.17	108.20
2	B	256	ARG	NE-CZ-NH1	13.43	127.02	120.30
2	B	324	ARG	NE-CZ-NH1	13.31	126.96	120.30
4	D	74	C	N3-C4-C5	-13.27	116.59	121.90
4	D	39	A	N1-C6-N6	13.05	126.43	118.60
3	C	93	G	C6-N1-C2	-12.96	117.32	125.10
4	D	38	A	N1-C6-N6	-12.82	110.91	118.60
1	A	198	ARG	NE-CZ-NH1	12.75	126.67	120.30
1	A	194	ARG	NE-CZ-NH1	12.51	126.56	120.30
4	D	1	G	C5-C6-O6	-12.42	121.15	128.60
4	D	73	C	N3-C4-C5	-12.35	116.96	121.90
4	D	49	C	N3-C4-C5	-12.13	117.05	121.90
4	D	64	G	N1-C6-O6	12.10	127.16	119.90
4	D	16	C	O4'-C1'-N1	12.09	117.87	108.20
4	D	11	C	N3-C4-C5	-11.99	117.11	121.90
4	D	16	C	P-O3'-C3'	11.96	134.06	119.70
4	D	1	G	N1-C6-O6	11.94	127.06	119.90
1	A	81	ARG	NE-CZ-NH1	11.93	126.26	120.30
3	C	92	U	O4'-C1'-N1	11.76	117.60	108.20
4	D	23	A	C2-N3-C4	-11.66	104.77	110.60
4	D	79	C	O4'-C1'-N1	11.62	117.50	108.20
1	A	47	ARG	NE-CZ-NH1	11.58	126.09	120.30
3	C	96	A	C8-N9-C4	11.52	110.41	105.80
1	A	402	PHE	CB-CG-CD1	-11.48	112.77	120.80
4	D	45	C	O4'-C1'-N1	11.41	117.33	108.20
4	D	56	G	C4-C5-N7	-11.34	106.26	110.80
4	D	71	A	N1-C6-N6	11.30	125.38	118.60
1	A	303	PHE	CB-CG-CD2	-11.27	112.91	120.80
4	D	53	A	C2-N3-C4	-11.20	105.00	110.60
4	D	62	G	N7-C8-N9	-11.19	107.50	113.10
4	D	13	G	C5-C6-O6	-11.11	121.94	128.60
4	D	4	G	N1-C6-O6	11.08	126.55	119.90
4	D	69	G	C5-C6-O6	-11.07	121.96	128.60
4	D	87	C	C6-N1-C2	-11.05	115.88	120.30
4	D	49	C	C5-C4-N4	10.96	127.87	120.20
4	D	70	A	N1-C6-N6	-10.92	112.05	118.60
4	D	70	A	P-O3'-C3'	10.90	132.78	119.70
4	D	45	C	N3-C4-C5	-10.80	117.58	121.90
2	B	240	ASP	CB-CG-OD2	-10.80	108.58	118.30
2	B	425	TYR	CB-CG-CD2	-10.68	114.59	121.00
4	D	5	G	C5-C6-O6	-10.59	122.25	128.60
4	D	40	G	C2-N3-C4	-10.57	106.62	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	39	A	C5-C6-N6	-10.55	115.26	123.70
4	D	56	G	C5-C6-O6	-10.55	122.27	128.60
4	D	37	C	C5-C6-N1	10.45	126.22	121.00
2	B	618	ARG	NE-CZ-NH1	10.35	125.48	120.30
4	D	44	C	O4'-C1'-N1	10.34	116.47	108.20
4	D	19	G	C5-C6-N1	10.33	116.67	111.50
4	D	35	C	N3-C4-C5	-10.31	117.78	121.90
4	D	61	C	O4'-C1'-N1	10.27	116.42	108.20
4	D	76	C	C2-N3-C4	-10.24	114.78	119.90
4	D	38	A	C4-C5-C6	-10.23	111.89	117.00
4	D	13	G	N7-C8-N9	-10.17	108.02	113.10
4	D	16	C	N3-C4-N4	-10.15	110.89	118.00
4	D	56	G	N1-C6-O6	10.13	125.98	119.90
4	D	85	A	P-O3'-C3'	-10.11	107.56	119.70
2	B	448	TYR	CB-CG-CD1	-10.10	114.94	121.00
1	A	357	PHE	CB-CG-CD1	-10.09	113.74	120.80
4	D	74	C	O4'-C1'-N1	10.09	116.27	108.20
4	D	85	A	C8-N9-C4	-10.06	101.78	105.80
2	B	432	PHE	CB-CG-CD1	-10.04	113.78	120.80
4	D	8	U	C5-C6-N1	-10.01	117.69	122.70
4	D	68	C	N3-C4-C5	9.95	125.88	121.90
4	D	86	C	N3-C4-C5	-9.89	117.94	121.90
4	D	83	G	C5-C6-O6	-9.85	122.69	128.60
1	A	240	ASP	CB-CG-OD1	9.83	127.14	118.30
4	D	14	A	C8-N9-C4	9.82	109.73	105.80
4	D	35	C	N3-C4-N4	9.79	124.86	118.00
4	D	38	A	C6-N1-C2	-9.79	112.73	118.60
4	D	20	G	N1-C2-N2	-9.77	107.41	116.20
2	B	371	ARG	NE-CZ-NH2	-9.75	115.42	120.30
4	D	77	G	N1-C6-O6	9.71	125.72	119.90
4	D	46	C	N1-C2-O2	9.69	124.71	118.90
4	D	86	C	C4-C5-C6	9.69	122.24	117.40
4	D	3	G	C5-C6-O6	-9.68	122.79	128.60
4	D	73	C	N3-C4-N4	9.56	124.69	118.00
4	D	40	G	C8-N9-C4	9.55	110.22	106.40
4	D	28	C	O4'-C1'-N1	9.53	115.82	108.20
4	D	85	A	N7-C8-N9	9.51	118.55	113.80
2	B	339	ARG	NE-CZ-NH1	9.50	125.05	120.30
3	C	92	U	N3-C4-C5	-9.50	108.90	114.60
4	D	85	A	O4'-C1'-N9	9.46	115.77	108.20
4	D	9	U	P-O3'-C3'	9.37	130.95	119.70
2	B	583	ARG	NE-CZ-NH2	-9.35	115.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	PHE	CB-CG-CD2	-9.34	114.26	120.80
1	A	201	TYR	CB-CG-CD1	-9.17	115.50	121.00
4	D	56	G	N9-C4-C5	9.11	109.04	105.40
1	A	85	TYR	CB-CG-CD1	9.09	126.45	121.00
4	D	70	A	C5-C6-N6	9.07	130.96	123.70
2	B	596	ARG	NE-CZ-NH2	-9.07	115.76	120.30
4	D	19	G	C4-C5-N7	9.06	114.43	110.80
4	D	22	C	P-O3'-C3'	9.05	130.56	119.70
4	D	32	G	O4'-C1'-N9	9.02	115.41	108.20
4	D	75	C	N3-C4-N4	8.98	124.28	118.00
4	D	22	C	O4'-C1'-N1	8.96	115.37	108.20
4	D	23	A	N7-C8-N9	-8.91	109.34	113.80
1	A	416	ARG	NE-CZ-NH2	-8.87	115.86	120.30
4	D	15	G	N3-C2-N2	-8.79	113.74	119.90
4	D	66	U	N3-C4-O4	-8.78	113.25	119.40
4	D	23	A	O4'-C1'-N9	8.74	115.19	108.20
1	A	258	TYR	CB-CG-CD2	8.65	126.19	121.00
2	B	249	ARG	NE-CZ-NH1	8.61	124.60	120.30
4	D	31	G	C1'-O4'-C4'	-8.60	103.02	109.90
4	D	16	C	N3-C4-C5	8.60	125.34	121.90
4	D	20	G	C2-N3-C4	-8.58	107.61	111.90
1	A	158	PHE	CB-CG-CD2	-8.58	114.79	120.80
4	D	15	G	O4'-C1'-N9	8.55	115.04	108.20
4	D	19	G	P-O3'-C3'	8.52	129.93	119.70
4	D	84	C	O4'-C1'-N1	8.49	114.99	108.20
4	D	35	C	N3-C2-O2	-8.48	115.96	121.90
4	D	4	G	C5-C6-O6	-8.47	123.52	128.60
4	D	33	G	C2-N3-C4	8.47	116.14	111.90
4	D	57	G	C8-N9-C4	-8.46	103.02	106.40
4	D	65	G	C5-C6-O6	-8.40	123.56	128.60
4	D	3	G	C4-C5-N7	8.37	114.15	110.80
1	A	152	ASP	CB-CG-OD1	8.36	125.82	118.30
4	D	42	U	C6-N1-C2	-8.35	115.99	121.00
4	D	83	G	O4'-C1'-N9	8.34	114.87	108.20
1	A	240	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	A	55	GLU	OE1-CD-OE2	8.27	133.22	123.30
4	D	40	G	N3-C4-C5	8.27	132.73	128.60
4	D	84	C	N3-C4-C5	-8.27	118.59	121.90
3	C	98	A	N1-C6-N6	-8.26	113.64	118.60
4	D	22	C	C6-N1-C2	8.24	123.60	120.30
1	A	10	ARG	NE-CZ-NH2	8.20	124.40	120.30
4	D	49	C	O4'-C1'-N1	8.19	114.75	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	417	TYR	CB-CG-CD2	8.16	125.90	121.00
2	B	272	ARG	NE-CZ-NH1	8.13	124.37	120.30
4	D	32	G	C8-N9-C4	-8.13	103.15	106.40
1	A	56	PHE	CB-CG-CD1	-8.13	115.11	120.80
4	D	86	C	N3-C4-N4	8.12	123.68	118.00
4	D	49	C	C2-N3-C4	8.12	123.96	119.90
4	D	29	G	N3-C2-N2	8.11	125.58	119.90
4	D	79	C	C6-N1-C2	-8.08	117.07	120.30
4	D	39	A	N1-C2-N3	-8.04	125.28	129.30
4	D	29	G	C4-C5-N7	-8.01	107.59	110.80
4	D	70	A	C4-C5-C6	-7.97	113.01	117.00
4	D	76	C	N3-C4-C5	7.97	125.09	121.90
2	B	324	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	289	ARG	NE-CZ-NH2	-7.94	116.33	120.30
4	D	40	G	N9-C4-C5	-7.93	102.23	105.40
4	D	51	G	N3-C2-N2	7.93	125.45	119.90
3	C	96	A	N9-C4-C5	-7.92	102.63	105.80
1	A	56	PHE	CB-CG-CD2	7.92	126.34	120.80
4	D	88	A	C6-N1-C2	-7.91	113.85	118.60
4	D	6	G	C6-N1-C2	-7.91	120.35	125.10
2	B	332	PHE	CB-CG-CD1	7.89	126.32	120.80
4	D	20	G	C1'-O4'-C4'	-7.89	103.59	109.90
4	D	65	G	N1-C6-O6	7.89	124.63	119.90
4	D	53	A	N1-C2-N3	7.85	133.23	129.30
4	D	8	U	C4-C5-C6	7.85	124.41	119.70
1	A	47	ARG	NE-CZ-NH2	-7.83	116.39	120.30
4	D	54	G	N9-C4-C5	-7.82	102.27	105.40
4	D	63	G	O4'-C1'-N9	7.80	114.44	108.20
4	D	14	A	N7-C8-N9	-7.77	109.91	113.80
4	D	60	C	P-O3'-C3'	7.77	129.03	119.70
4	D	74	C	N3-C4-N4	7.75	123.42	118.00
1	A	255	ASP	CB-CG-OD2	7.75	125.27	118.30
4	D	69	G	N1-C6-O6	7.71	124.53	119.90
4	D	76	C	N3-C2-O2	-7.70	116.51	121.90
3	C	96	A	N7-C8-N9	-7.67	109.96	113.80
2	B	371	ARG	NE-CZ-NH1	7.66	124.13	120.30
4	D	75	C	O4'-C1'-N1	7.66	114.33	108.20
4	D	63	G	N9-C4-C5	7.64	108.46	105.40
4	D	74	C	N3-C2-O2	-7.64	116.55	121.90
1	A	203	ARG	NH1-CZ-NH2	7.64	127.81	119.40
1	A	182	ARG	NE-CZ-NH2	-7.64	116.48	120.30
4	D	55	G	C5-N7-C8	-7.63	100.49	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	62	G	C5-N7-C8	7.60	108.10	104.30
2	B	516	PHE	CB-CG-CD1	7.58	126.10	120.80
4	D	46	C	C5-C4-N4	7.57	125.50	120.20
2	B	618	ARG	NE-CZ-NH2	-7.57	116.52	120.30
3	C	96	A	N1-C6-N6	-7.56	114.06	118.60
4	D	12	C	O4'-C1'-N1	7.56	114.25	108.20
4	D	11	C	O4'-C1'-N1	7.56	114.25	108.20
4	D	6	G	C2-N3-C4	7.53	115.67	111.90
4	D	40	G	N3-C2-N2	-7.52	114.63	119.90
4	D	25	A	C2-N3-C4	7.52	114.36	110.60
4	D	52	U	OP1-P-OP2	-7.52	108.32	119.60
4	D	46	C	N3-C2-O2	-7.45	116.68	121.90
4	D	19	G	C3'-C2'-C1'	7.45	107.46	101.50
4	D	28	C	N1-C2-O2	7.45	123.37	118.90
1	A	148	PHE	CB-CG-CD2	-7.40	115.62	120.80
4	D	62	G	O4'-C1'-N9	7.40	114.12	108.20
1	A	194	ARG	NE-CZ-NH2	-7.39	116.61	120.30
4	D	57	G	C5-C6-O6	7.39	133.03	128.60
4	D	4	G	C4-C5-N7	-7.38	107.85	110.80
2	B	217	PHE	CB-CG-CD1	-7.34	115.66	120.80
4	D	46	C	N3-C4-C5	-7.34	118.96	121.90
4	D	52	U	P-O5'-C5'	7.33	132.63	120.90
4	D	21	U	O4'-C1'-N1	7.33	114.06	108.20
4	D	43	C	O5'-P-OP1	-7.31	99.12	105.70
4	D	14	A	P-O5'-C5'	7.29	132.56	120.90
4	D	5	G	N1-C6-O6	7.28	124.27	119.90
4	D	22	C	C4-C5-C6	-7.28	113.76	117.40
4	D	14	A	N1-C6-N6	7.28	122.97	118.60
4	D	74	C	C6-N1-C2	-7.23	117.41	120.30
4	D	77	G	C5-C6-N1	-7.22	107.89	111.50
2	B	432	PHE	CB-CG-CD2	7.22	125.86	120.80
4	D	52	U	O4'-C1'-N1	7.20	113.96	108.20
3	C	93	G	C5-C6-N1	7.20	115.10	111.50
3	C	92	U	C2-N3-C4	7.18	131.31	127.00
4	D	26	G	N9-C4-C5	-7.16	102.54	105.40
1	A	291	PHE	CB-CG-CD2	-7.16	115.79	120.80
4	D	73	C	C4'-C3'-C2'	-7.15	95.45	102.60
4	D	43	C	C5-C4-N4	-7.14	115.20	120.20
4	D	53	A	C4-C5-N7	7.13	114.27	110.70
3	C	98	A	C4-C5-N7	-7.12	107.14	110.70
2	B	240	ASP	CB-CG-OD1	7.12	124.70	118.30
1	A	158	PHE	CB-CG-CD1	7.11	125.78	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	39	A	P-O3'-C3'	7.11	128.23	119.70
4	D	47	U	C2-N3-C4	-7.10	122.74	127.00
2	B	482	LEU	O-C-N	-7.09	111.14	123.20
1	A	166	ARG	NH1-CZ-NH2	-7.09	111.60	119.40
4	D	29	G	C5-N7-C8	7.09	107.84	104.30
1	A	414	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	314	MET	CG-SD-CE	-6.99	89.02	100.20
3	C	98	A	C6-N1-C2	-6.99	114.41	118.60
4	D	5	G	C8-N9-C4	6.98	109.19	106.40
4	D	31	G	C4'-C3'-C2'	-6.97	95.62	102.60
4	D	7	G	C5-C6-N1	-6.97	108.02	111.50
4	D	75	C	N3-C4-C5	-6.96	119.12	121.90
4	D	77	G	O4'-C1'-N9	6.96	113.77	108.20
4	D	71	A	C5-C6-N6	-6.95	118.14	123.70
3	C	91	U	N1-C2-N3	-6.95	110.73	114.90
4	D	57	G	N3-C4-C5	-6.94	125.13	128.60
1	A	81	ARG	NH1-CZ-NH2	-6.93	111.78	119.40
4	D	61	C	C5-C6-N1	-6.93	117.54	121.00
4	D	24	A	N9-C4-C5	6.92	108.57	105.80
2	B	282	ARG	NE-CZ-NH1	6.92	123.76	120.30
4	D	54	G	C4-C5-N7	6.92	113.57	110.80
4	D	30	G	C5-C6-O6	-6.91	124.46	128.60
4	D	19	G	C6-N1-C2	-6.89	120.97	125.10
4	D	70	A	C5-N7-C8	-6.88	100.46	103.90
2	B	256	ARG	NE-CZ-NH2	-6.87	116.86	120.30
2	B	286	GLU	OE1-CD-OE2	-6.85	115.08	123.30
4	D	20	G	N1-C2-N3	6.85	128.01	123.90
2	B	481	VAL	O-C-N	-6.84	111.75	122.70
4	D	13	G	C5-C6-N1	-6.83	108.09	111.50
4	D	26	G	O4'-C1'-N9	6.82	113.66	108.20
2	B	520	ASP	CA-CB-CG	6.80	128.37	113.40
1	A	174	VAL	CG1-CB-CG2	-6.80	100.03	110.90
4	D	37	C	C4-C5-C6	-6.79	114.01	117.40
4	D	45	C	C2-N3-C4	6.78	123.29	119.90
2	B	208	PRO	N-CA-CB	6.77	111.42	103.30
4	D	15	G	C6-N1-C2	-6.77	121.04	125.10
4	D	43	C	N3-C4-N4	6.75	122.73	118.00
4	D	33	G	C5-N7-C8	-6.75	100.93	104.30
2	B	362	ASP	CB-CG-OD2	6.74	124.37	118.30
4	D	88	A	C1'-O4'-C4'	-6.74	104.51	109.90
4	D	35	C	C6-N1-C1'	6.72	128.87	120.80
1	A	85	TYR	CB-CG-CD2	-6.72	116.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	13	G	C5-N7-C8	6.70	107.65	104.30
4	D	52	U	N1-C2-N3	-6.70	110.88	114.90
2	B	434	ARG	NE-CZ-NH1	6.69	123.65	120.30
4	D	28	C	C5-C6-N1	6.69	124.35	121.00
4	D	76	C	N1-C2-O2	6.69	122.91	118.90
4	D	4	G	O4'-C1'-N9	6.68	113.55	108.20
1	A	264	PHE	CB-CG-CD1	6.67	125.47	120.80
4	D	34	A	P-O3'-C3'	6.67	127.70	119.70
4	D	35	C	C1'-O4'-C4'	-6.66	104.57	109.90
4	D	16	C	C4-C5-C6	-6.65	114.08	117.40
4	D	25	A	P-O3'-C3'	-6.65	111.72	119.70
2	B	530	THR	OG1-CB-CG2	-6.64	94.72	110.00
1	A	66	VAL	CA-CB-CG2	-6.64	100.94	110.90
3	C	94	U	O4'-C1'-N1	6.64	113.51	108.20
4	D	53	A	C6-C5-N7	-6.64	127.65	132.30
1	A	245	ARG	NE-CZ-NH1	6.63	123.61	120.30
4	D	74	C	N1-C2-N3	6.62	123.84	119.20
4	D	78	C	C6-N1-C2	-6.61	117.66	120.30
4	D	8	U	N3-C4-C5	-6.60	110.64	114.60
2	B	249	ARG	NE-CZ-NH2	-6.60	117.00	120.30
4	D	37	C	N1-C2-O2	-6.59	114.94	118.90
4	D	19	G	N1-C6-O6	-6.59	115.95	119.90
4	D	49	C	C5'-C4'-O4'	6.59	117.01	109.10
4	D	55	G	C6-C5-N7	-6.58	126.45	130.40
2	B	451	MET	CG-SD-CE	-6.58	89.67	100.20
4	D	39	A	N3-C4-N9	-6.57	122.14	127.40
4	D	49	C	N1-C2-O2	6.57	122.84	118.90
4	D	22	C	N3-C2-O2	6.57	126.50	121.90
2	B	596	ARG	NE-CZ-NH1	6.55	123.58	120.30
3	C	94	U	C4-C5-C6	6.55	123.63	119.70
4	D	14	A	C5-C6-N6	-6.52	118.48	123.70
4	D	37	C	N1-C2-N3	6.52	123.76	119.20
4	D	2	C	C3'-C2'-C1'	-6.50	96.30	101.50
4	D	1	G	O4'-C1'-N9	6.50	113.40	108.20
4	D	50	C	C5-C6-N1	-6.50	117.75	121.00
4	D	86	C	O4'-C1'-N1	6.49	113.39	108.20
4	D	83	G	N7-C8-N9	6.49	116.35	113.10
4	D	88	A	O4'-C1'-N9	6.48	113.38	108.20
1	A	74	ALA	CB-CA-C	-6.47	100.39	110.10
4	D	87	C	C5-C6-N1	6.47	124.24	121.00
1	A	257	SER	O-C-N	-6.45	112.38	122.70
4	D	57	G	C4-C5-N7	-6.45	108.22	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	38	A	C1'-O4'-C4'	6.45	115.06	109.90
2	B	434	ARG	NE-CZ-NH2	-6.44	117.08	120.30
4	D	77	G	C2-N3-C4	6.44	115.12	111.90
1	A	28	ARG	C-N-CA	6.43	135.80	122.30
2	B	258	THR	CA-CB-CG2	-6.42	103.41	112.40
4	D	55	G	C5-C6-O6	-6.42	124.75	128.60
4	D	71	A	C2-N3-C4	-6.41	107.39	110.60
4	D	43	C	C6-N1-C2	-6.38	117.75	120.30
4	D	73	C	C4-C5-C6	6.37	120.58	117.40
1	A	137	THR	N-CA-CB	6.36	122.39	110.30
4	D	69	G	C6-N1-C2	-6.34	121.30	125.10
4	D	33	G	N9-C4-C5	6.33	107.93	105.40
4	D	88	A	C5-C6-N1	6.32	120.86	117.70
4	D	13	G	N3-C2-N2	6.32	124.32	119.90
3	C	98	A	N9-C4-C5	6.32	108.33	105.80
4	D	7	G	N1-C6-O6	6.30	123.68	119.90
4	D	54	G	N3-C2-N2	-6.30	115.49	119.90
4	D	70	A	N7-C8-N9	6.30	116.95	113.80
4	D	3	G	N1-C6-O6	6.29	123.67	119.90
4	D	37	C	O4'-C1'-N1	6.29	113.23	108.20
4	D	60	C	C6-N1-C2	-6.27	117.79	120.30
4	D	60	C	C2'-C3'-O3'	6.26	123.72	113.70
4	D	80	C	C5-C4-N4	6.26	124.58	120.20
4	D	1	G	C8-N9-C4	-6.25	103.90	106.40
1	A	402	PHE	CB-CG-CD2	6.25	125.17	120.80
4	D	7	G	C4-C5-C6	6.25	122.55	118.80
4	D	15	G	C8-N9-C4	-6.25	103.90	106.40
4	D	26	G	C2-N3-C4	-6.24	108.78	111.90
4	D	57	G	N9-C4-C5	6.24	107.90	105.40
4	D	85	A	O4'-C4'-C3'	-6.24	97.76	104.00
4	D	20	G	C8-N9-C4	-6.24	103.91	106.40
4	D	38	A	C5-C6-N6	6.24	128.69	123.70
4	D	73	C	P-O5'-C5'	-6.23	110.93	120.90
3	C	91	U	C2-N3-C4	-6.22	123.27	127.00
4	D	8	U	O4'-C1'-N1	6.21	113.17	108.20
1	A	148	PHE	CB-CG-CD1	6.21	125.14	120.80
4	D	24	A	O3'-P-O5'	-6.20	92.21	104.00
4	D	83	G	C4-N9-C1'	6.20	134.55	126.50
4	D	43	C	C6-N1-C1'	6.19	128.23	120.80
1	A	37	LEU	CB-CG-CD2	-6.18	100.50	111.00
4	D	68	C	N3-C4-N4	-6.17	113.68	118.00
4	D	5	G	N1-C2-N3	-6.16	120.20	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	62	G	N3-C2-N2	6.16	124.21	119.90
2	B	244	LEU	CB-CG-CD1	6.15	121.45	111.00
1	A	219	VAL	CG1-CB-CG2	6.14	120.73	110.90
4	D	48	C	O4'-C1'-N1	6.14	113.11	108.20
3	C	93	G	N1-C6-O6	-6.12	116.23	119.90
4	D	65	G	C5'-C4'-O4'	-6.12	101.76	109.10
3	C	97	A	N1-C2-N3	-6.11	126.24	129.30
4	D	2	C	O4'-C1'-N1	6.11	113.09	108.20
4	D	50	C	C6-N1-C2	6.10	122.74	120.30
1	A	309	LEU	CB-CG-CD1	6.08	121.34	111.00
3	C	91	U	C2'-C3'-O3'	6.08	123.43	113.70
4	D	54	G	C5-C6-O6	6.08	132.25	128.60
2	B	280	VAL	CG1-CB-CG2	-6.08	101.17	110.90
4	D	49	C	C4-C5-C6	6.08	120.44	117.40
4	D	25	A	C5-N7-C8	6.07	106.94	103.90
4	D	82	C	C3'-C2'-C1'	6.07	106.36	101.50
3	C	97	A	C6-C5-N7	6.06	136.54	132.30
4	D	74	C	C2-N1-C1'	6.06	125.47	118.80
4	D	36	U	C5'-C4'-O4'	6.05	116.36	109.10
1	A	245	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	B	516	PHE	CB-CG-CD2	-6.04	116.57	120.80
4	D	28	C	C4-C5-C6	-6.03	114.38	117.40
1	A	242	PHE	CB-CG-CD1	6.03	125.02	120.80
4	D	11	C	C2-N3-C4	6.03	122.92	119.90
2	B	272	ARG	NE-CZ-NH2	-6.03	117.28	120.30
4	D	7	G	P-O3'-C3'	6.02	126.92	119.70
4	D	29	G	N3-C4-N9	6.01	129.61	126.00
4	D	61	C	C4-C5-C6	6.01	120.41	117.40
4	D	26	G	C4-N9-C1'	-6.00	118.69	126.50
4	D	11	C	C4-C5-C6	6.00	120.40	117.40
4	D	25	A	N9-C4-C5	5.98	108.19	105.80
2	B	446	ASP	CB-CG-OD2	-5.98	112.92	118.30
4	D	14	A	O4'-C1'-N9	5.98	112.98	108.20
2	B	495	ALA	N-CA-CB	-5.97	101.74	110.10
4	D	26	G	C8-N9-C4	5.96	108.78	106.40
4	D	84	C	C5-C6-N1	-5.96	118.02	121.00
1	A	172	PHE	CB-CG-CD1	-5.95	116.63	120.80
4	D	9	U	C3'-C2'-C1'	5.95	106.26	101.50
4	D	36	U	O4'-C1'-N1	5.95	112.96	108.20
4	D	74	C	C4'-C3'-C2'	-5.94	96.66	102.60
4	D	33	G	C5-C6-O6	-5.94	125.04	128.60
3	C	93	G	N3-C4-N9	-5.94	122.44	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	29	G	O4'-C1'-N9	5.93	112.94	108.20
1	A	348	PRO	N-CA-CB	5.92	110.41	103.30
1	A	43	ASP	CB-CG-OD2	5.91	123.62	118.30
4	D	62	G	C4-C5-N7	-5.91	108.44	110.80
2	B	226	SER	N-CA-CB	5.91	119.36	110.50
4	D	41	A	N1-C2-N3	5.91	132.25	129.30
2	B	563	ILE	CA-CB-CG2	-5.90	99.09	110.90
2	B	538	ILE	CA-CB-CG2	-5.89	99.12	110.90
4	D	23	A	C5-C6-N1	-5.89	114.76	117.70
1	A	340	GLU	CA-CB-CG	5.88	126.34	113.40
4	D	12	C	N3-C4-C5	-5.88	119.55	121.90
4	D	61	C	N3-C4-N4	5.88	122.12	118.00
4	D	84	C	C6-N1-C1'	-5.88	113.74	120.80
3	C	98	A	P-O5'-C5'	5.88	130.31	120.90
1	A	295	SER	O-C-N	-5.86	113.32	122.70
3	C	90	A	C6-C5-N7	-5.86	128.20	132.30
4	D	24	A	N7-C8-N9	-5.85	110.88	113.80
4	D	21	U	P-O3'-C3'	5.85	126.72	119.70
4	D	41	A	C4-C5-N7	-5.85	107.78	110.70
4	D	80	C	C5'-C4'-O4'	5.84	116.11	109.10
4	D	7	G	C8-N9-C4	5.84	108.73	106.40
4	D	83	G	N1-C6-O6	5.84	123.40	119.90
4	D	72	U	P-O5'-C5'	-5.83	111.57	120.90
4	D	70	A	C4-C5-N7	5.83	113.61	110.70
2	B	622	LYS	N-CA-CB	-5.82	100.12	110.60
4	D	21	U	P-O5'-C5'	-5.82	111.58	120.90
4	D	63	G	C4-C5-N7	-5.82	108.47	110.80
2	B	272	ARG	CD-NE-CZ	-5.82	115.46	123.60
2	B	275	GLY	CA-C-O	-5.82	110.13	120.60
2	B	522	ASN	CB-CA-C	5.82	122.03	110.40
4	D	53	A	C5-N7-C8	-5.81	100.99	103.90
4	D	26	G	C3'-C2'-C1'	-5.80	96.86	101.50
1	A	51	MET	N-CA-CB	5.80	121.04	110.60
4	D	46	C	C6-N1-C2	5.80	122.62	120.30
2	B	616	THR	CA-CB-CG2	-5.80	104.28	112.40
4	D	88	A	N9-C4-C5	-5.80	103.48	105.80
4	D	35	C	N1-C2-N3	5.79	123.26	119.20
3	C	95	A	N1-C6-N6	5.79	122.07	118.60
2	B	608	ASP	CB-CG-OD1	-5.78	113.10	118.30
2	B	247	TYR	CB-CG-CD2	-5.78	117.53	121.00
4	D	46	C	OP1-P-OP2	-5.78	110.94	119.60
1	A	192	ARG	N-CA-C	5.76	126.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	69	G	C1'-O4'-C4'	-5.76	105.29	109.90
1	A	217	ASP	CB-CG-OD2	5.76	123.48	118.30
2	B	367	TRP	CZ3-CH2-CZ2	-5.76	114.69	121.60
4	D	65	G	C1'-O4'-C4'	-5.76	105.29	109.90
4	D	20	G	C6-N1-C2	-5.75	121.65	125.10
4	D	62	G	P-O5'-C5'	5.75	130.09	120.90
2	B	455	VAL	CB-CA-C	-5.74	100.49	111.40
4	D	9	U	C5-C6-N1	5.74	125.57	122.70
4	D	18	U	N3-C4-O4	-5.74	115.38	119.40
4	D	7	G	C8-N9-C1'	-5.73	119.55	127.00
4	D	37	C	C2-N3-C4	-5.72	117.04	119.90
4	D	35	C	O4'-C1'-N1	5.72	112.78	108.20
2	B	417	TYR	CG-CD1-CE1	5.72	125.87	121.30
4	D	23	A	C5-N7-C8	5.71	106.76	103.90
4	D	52	U	N3-C2-O2	5.71	126.19	122.20
4	D	44	C	O4'-C4'-C3'	-5.71	98.29	104.00
2	B	330	THR	CA-CB-CG2	-5.70	104.41	112.40
4	D	8	U	C5'-C4'-O4'	5.69	115.93	109.10
4	D	35	C	C2-N1-C1'	-5.69	112.54	118.80
4	D	84	C	C3'-C2'-C1'	5.68	106.04	101.50
4	D	19	G	N3-C2-N2	5.67	123.87	119.90
4	D	30	G	C5-C6-N1	5.67	114.34	111.50
4	D	75	C	C5-C4-N4	-5.67	116.23	120.20
4	D	42	U	P-O5'-C5'	5.67	129.98	120.90
4	D	41	A	C4-C5-C6	5.67	119.83	117.00
3	C	95	A	O4'-C1'-N9	5.66	112.73	108.20
3	C	92	U	N3-C2-O2	5.66	126.16	122.20
4	D	30	G	C3'-C2'-C1'	-5.66	96.97	101.50
4	D	57	G	C4'-C3'-C2'	-5.66	96.94	102.60
2	B	448	TYR	CG-CD1-CE1	-5.66	116.78	121.30
4	D	85	A	C5'-C4'-O4'	5.65	115.88	109.10
2	B	449	LYS	CB-CA-C	5.64	121.69	110.40
4	D	51	G	C2'-C3'-O3'	5.64	122.72	113.70
4	D	79	C	N3-C2-O2	-5.64	117.95	121.90
4	D	34	A	O4'-C1'-C2'	5.62	112.66	107.60
4	D	49	C	N3-C2-O2	-5.62	117.97	121.90
2	B	489	VAL	CA-CB-CG2	5.61	119.31	110.90
4	D	31	G	N7-C8-N9	-5.61	110.30	113.10
4	D	87	C	C4'-C3'-C2'	-5.61	96.99	102.60
4	D	66	U	C5-C4-O4	5.60	129.26	125.90
4	D	76	C	C3'-C2'-C1'	-5.60	97.02	101.50
1	A	113	ASP	N-CA-CB	5.58	120.65	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	30	G	N3-C4-N9	-5.57	122.66	126.00
2	B	522	ASN	O-C-N	-5.57	113.79	122.70
4	D	10	G	O4'-C1'-N9	5.57	112.66	108.20
4	D	32	G	N3-C2-N2	5.57	123.80	119.90
3	C	98	A	N1-C2-N3	5.57	132.08	129.30
4	D	40	G	C5'-C4'-C3'	-5.57	107.10	116.00
2	B	367	TRP	CH2-CZ2-CE2	5.56	122.96	117.40
3	C	92	U	C4-C5-C6	5.56	123.04	119.70
3	C	99	A	N7-C8-N9	-5.56	111.02	113.80
4	D	16	C	N3-C2-O2	-5.56	118.01	121.90
1	A	377	TRP	CB-CG-CD2	-5.55	119.39	126.60
1	A	267	ALA	CB-CA-C	-5.54	101.80	110.10
2	B	598	ALA	C-N-CA	5.53	133.90	122.30
4	D	32	G	OP2-P-O3'	5.53	117.35	105.20
4	D	71	A	C8-N9-C4	-5.50	103.60	105.80
4	D	15	G	C5-N7-C8	5.50	107.05	104.30
4	D	48	C	C5'-C4'-C3'	5.50	124.80	116.00
4	D	83	G	P-O3'-C3'	5.50	126.30	119.70
2	B	380	VAL	CA-CB-CG2	-5.49	102.66	110.90
4	D	26	G	C4-C5-N7	5.49	113.00	110.80
4	D	34	A	N9-C4-C5	-5.49	103.61	105.80
3	C	95	A	P-O5'-C5'	5.48	129.67	120.90
4	D	36	U	C4-C5-C6	-5.48	116.41	119.70
4	D	83	G	C8-N9-C4	-5.48	104.21	106.40
4	D	3	G	C5-N7-C8	-5.48	101.56	104.30
1	A	276	SER	O-C-N	-5.47	113.94	122.70
1	A	128	ASP	N-CA-CB	-5.47	100.75	110.60
4	D	38	A	O4'-C1'-N9	5.46	112.56	108.20
2	B	506	GLY	O-C-N	-5.45	113.98	122.70
1	A	412	ILE	C-N-CA	5.44	135.31	121.70
4	D	55	G	N1-C6-O6	5.44	123.17	119.90
2	B	332	PHE	CG-CD2-CE2	5.44	126.79	120.80
1	A	239	SER	O-C-N	-5.44	114.00	122.70
1	A	335	CYS	CA-CB-SG	5.44	123.79	114.00
2	B	448	TYR	CB-CG-CD2	5.44	124.26	121.00
2	B	217	PHE	CB-CG-CD2	5.42	124.60	120.80
2	B	234	TYR	CG-CD2-CE2	-5.41	116.97	121.30
4	D	66	U	P-O5'-C5'	5.41	129.56	120.90
4	D	88	A	C5-C6-N6	-5.40	119.38	123.70
4	D	7	G	C5'-C4'-O4'	5.40	115.58	109.10
3	C	92	U	C5-C4-O4	5.40	129.14	125.90
1	A	131	PHE	CB-CG-CD1	5.40	124.58	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	250	GLU	CA-CB-CG	5.38	125.24	113.40
1	A	389	LEU	CB-CG-CD2	5.37	120.13	111.00
1	A	290	TYR	CB-CA-C	5.36	121.12	110.40
3	C	96	A	C8-N9-C1'	-5.36	118.05	127.70
4	D	24	A	N1-C2-N3	-5.36	126.62	129.30
4	D	23	A	N3-C4-N9	-5.35	123.12	127.40
1	A	385	PHE	CB-CG-CD2	5.35	124.55	120.80
4	D	27	G	C5-N7-C8	-5.34	101.63	104.30
2	B	548	TYR	CD1-CE1-CZ	5.33	124.59	119.80
4	D	54	G	P-O3'-C3'	5.33	126.09	119.70
1	A	78	VAL	CA-CB-CG1	5.32	118.88	110.90
4	D	76	C	O5'-P-OP1	5.32	117.08	110.70
4	D	54	G	N3-C4-C5	5.32	131.26	128.60
2	B	551	VAL	CA-CB-CG1	-5.31	102.93	110.90
2	B	242	ARG	NE-CZ-NH2	-5.31	117.64	120.30
4	D	51	G	C2-N3-C4	5.31	114.55	111.90
4	D	42	U	C5-C6-N1	5.30	125.35	122.70
3	C	91	U	N1-C2-O2	5.29	126.51	122.80
4	D	69	G	C4-C5-C6	-5.29	115.63	118.80
4	D	3	G	C5'-C4'-C3'	5.29	124.46	116.00
2	B	536	VAL	N-CA-CB	5.29	123.13	111.50
4	D	80	C	C2-N3-C4	5.28	122.54	119.90
4	D	56	G	O4'-C1'-N9	5.28	112.42	108.20
4	D	57	G	C2-N3-C4	5.28	114.54	111.90
4	D	84	C	P-O5'-C5'	5.28	129.34	120.90
4	D	9	U	C5-C4-O4	-5.27	122.74	125.90
4	D	32	G	N7-C8-N9	5.27	115.73	113.10
4	D	11	C	C6-N1-C2	5.26	122.41	120.30
4	D	7	G	C6-C5-N7	-5.26	127.25	130.40
1	A	152	ASP	CB-CG-OD2	-5.25	113.57	118.30
4	D	9	U	N3-C4-O4	5.24	123.07	119.40
2	B	494	VAL	CG1-CB-CG2	-5.24	102.52	110.90
4	D	1	G	O3'-P-O5'	-5.24	94.05	104.00
4	D	70	A	C1'-O4'-C4'	5.24	114.09	109.90
3	C	97	A	C3'-C2'-C1'	-5.23	97.32	101.50
4	D	30	G	N9-C1'-C2'	-5.21	106.26	112.00
2	B	372	TYR	CZ-CE2-CD2	-5.21	115.11	119.80
4	D	47	U	OP1-P-OP2	-5.21	111.79	119.60
3	C	96	A	C1'-O4'-C4'	5.21	114.06	109.90
1	A	325	ASN	CA-CB-CG	-5.20	101.96	113.40
4	D	36	U	N3-C4-C5	5.20	117.72	114.60
2	B	529	ARG	NE-CZ-NH1	5.20	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	48	C	C6-N1-C2	-5.19	118.22	120.30
4	D	3	G	C8-N9-C1'	5.18	133.74	127.00
1	A	114	PHE	CB-CG-CD1	-5.18	117.17	120.80
1	A	88	VAL	CA-CB-CG2	-5.18	103.13	110.90
2	B	556	THR	CA-CB-CG2	-5.17	105.16	112.40
4	D	41	A	C5-N7-C8	5.17	106.49	103.90
1	A	355	SER	N-CA-CB	5.17	118.25	110.50
2	B	397	MET	CA-CB-CG	5.17	122.08	113.30
4	D	80	C	O4'-C1'-N1	5.16	112.33	108.20
1	A	241	MET	CG-SD-CE	-5.16	91.94	100.20
4	D	15	G	P-O3'-C3'	-5.16	113.51	119.70
3	C	94	U	C1'-O4'-C4'	-5.15	105.78	109.90
3	C	94	U	N3-C4-C5	-5.15	111.51	114.60
4	D	80	C	C4-C5-C6	5.15	119.97	117.40
4	D	7	G	O4'-C1'-N9	5.14	112.31	108.20
4	D	68	C	C4-C5-C6	-5.14	114.83	117.40
4	D	59	U	C1'-O4'-C4'	5.13	114.00	109.90
1	A	213	PHE	CD1-CE1-CZ	-5.12	113.95	120.10
2	B	442	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	A	10	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
2	B	605	THR	CA-CB-CG2	-5.10	105.26	112.40
1	A	355	SER	CB-CA-C	-5.10	100.41	110.10
4	D	31	G	O4'-C1'-C2'	5.09	112.19	107.60
1	A	101	VAL	CB-CA-C	5.09	121.07	111.40
4	D	48	C	C2-N3-C4	5.09	122.44	119.90
2	B	554	ILE	CA-CB-CG2	-5.08	100.73	110.90
4	D	16	C	C5-C4-N4	5.08	123.75	120.20
4	D	62	G	P-O3'-C3'	-5.07	113.61	119.70
4	D	41	A	C5'-C4'-O4'	5.07	115.19	109.10
1	A	58	THR	CA-CB-CG2	-5.07	105.31	112.40
4	D	65	G	C8-N9-C4	5.06	108.43	106.40
2	B	576	GLU	CB-CA-C	-5.06	100.28	110.40
4	D	6	G	C5-C6-O6	-5.06	125.56	128.60
4	D	20	G	P-O3'-C3'	-5.06	113.63	119.70
4	D	16	C	C2-N3-C4	-5.05	117.37	119.90
2	B	265	LEU	N-CA-CB	5.05	120.50	110.40
2	B	555	HIS	CA-CB-CG	5.05	122.19	113.60
1	A	146	PHE	CB-CG-CD2	-5.05	117.27	120.80
4	D	20	G	N3-C2-N2	5.05	123.43	119.90
4	D	34	A	O4'-C1'-N9	5.04	112.23	108.20
4	D	42	U	C5-C4-O4	5.04	128.93	125.90
4	D	32	G	C5-N7-C8	-5.04	101.78	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	82	C	O4'-C1'-N1	5.03	112.23	108.20
4	D	40	G	P-O5'-C5'	5.03	128.95	120.90
1	A	382	TYR	CG-CD1-CE1	-5.03	117.28	121.30
4	D	2	C	N3-C4-C5	-5.03	119.89	121.90
2	B	448	TYR	CG-CD2-CE2	-5.03	117.28	121.30
2	B	332	PHE	N-CA-CB	-5.02	101.57	110.60
2	B	380	VAL	CG1-CB-CG2	-5.02	102.87	110.90
4	D	70	A	O4'-C1'-N9	5.01	112.21	108.20
2	B	315	ASP	CB-CG-OD1	5.01	122.81	118.30
4	D	19	G	O3'-P-O5'	-5.01	94.48	104.00
4	D	7	G	C4'-C3'-C2'	5.01	107.61	102.60

There are no chirality outliers.

All (89) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	HIS	Sidechain
1	A	141	SER	Peptide
1	A	142	ASP	Peptide
1	A	144	SER	Peptide
1	A	194	ARG	Sidechain
1	A	275	LEU	Peptide
1	A	276	SER	Peptide
1	A	278	VAL	Peptide
1	A	28	ARG	Sidechain
1	A	301	TYR	Sidechain
1	A	323	TYR	Sidechain
1	A	325	ASN	Peptide
1	A	331	TYR	Sidechain
1	A	356	HIS	Sidechain
1	A	402	PHE	Sidechain
1	A	419	PHE	Sidechain
1	A	81	ARG	Sidechain
2	B	232	ILE	Mainchain
2	B	247	TYR	Sidechain
2	B	272	ARG	Sidechain
2	B	292	PHE	Peptide
2	B	303	PHE	Sidechain
2	B	314	ALA	Peptide
2	B	328	PHE	Sidechain
2	B	371	ARG	Sidechain
2	B	372	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	439	PRO	Peptide
2	B	448	TYR	Sidechain
2	B	469	GLN	Peptide
2	B	473	MET	Peptide
2	B	503	ARG	Sidechain
2	B	517	ILE	Peptide
2	B	521	PRO	Peptide
2	B	524	LEU	Peptide
2	B	528	GLY	Peptide
2	B	536	VAL	Peptide
2	B	539	GLU	Peptide
2	B	553	HIS	Sidechain
2	B	581	ARG	Sidechain
2	B	583	ARG	Sidechain
3	C	90	A	Sidechain
3	C	91	U	Sidechain
3	C	92	U	Sidechain
3	C	93	G	Sidechain
3	C	95	A	Sidechain
3	C	97	A	Sidechain
3	C	98	A	Sidechain
4	D	1	G	Sidechain
4	D	10	G	Sidechain
4	D	12	C	Sidechain
4	D	14	A	Sidechain
4	D	15	G	Sidechain
4	D	18	U	Sidechain
4	D	19	G	Sidechain
4	D	20	G	Sidechain
4	D	21	U	Sidechain
4	D	23	A	Sidechain
4	D	24	A	Sidechain
4	D	26	G	Sidechain
4	D	28	C	Sidechain
4	D	29	G	Sidechain
4	D	30	G	Sidechain
4	D	36	U	Sidechain
4	D	37	C	Sidechain
4	D	38	A	Sidechain
4	D	39	A	Sidechain
4	D	4	G	Sidechain
4	D	40	G	Sidechain

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Mol	Chain	Res	Type	Group
4	D	44	C	Sidechain
4	D	47	U	Sidechain
4	D	5	G	Sidechain
4	D	51	G	Sidechain
4	D	54	G	Sidechain
4	D	55	G	Sidechain
4	D	59	U	Sidechain
4	D	61	C	Sidechain
4	D	62	G	Sidechain
4	D	65	G	Sidechain
4	D	69	G	Sidechain
4	D	70	A	Sidechain
4	D	71	A	Sidechain
4	D	76	C	Sidechain
4	D	78	C	Sidechain
4	D	8	U	Sidechain
4	D	83	G	Sidechain
4	D	85	A	Sidechain
4	D	87	C	Sidechain
4	D	88	A	Sidechain
4	D	9	U	Sidechain

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3269	0	3314	10	0
2	B	3367	0	3424	11	0
3	C	212	0	106	8	0
4	D	1876	0	938	15	0
All	All	8724	0	7782	37	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:U:N3	4:D:39:A:N1	2.19	0.90
3:C:92:U:C2	4:D:38:A:C2	2.81	0.69
4:D:39:A:H3'	4:D:40:G:C8	2.30	0.67
2:B:308:ILE:HG21	2:B:553:HIS:CE1	2.34	0.63
2:B:617:LEU:HD23	2:B:625:ALA:HB3	1.84	0.57
1:A:15:TRP:CD1	1:A:19:LYS:HE2	2.39	0.57
3:C:91:U:C2	4:D:39:A:C2	2.93	0.57
3:C:92:U:O2	4:D:38:A:C2	2.62	0.52
3:C:91:U:C4	4:D:39:A:N1	2.76	0.52
1:A:274:VAL:HG12	1:A:274:VAL:O	2.13	0.48
4:D:15:G:H3'	4:D:16:C:H5''	1.96	0.47
4:D:1:G:C2	4:D:85:A:C2	3.02	0.47
2:B:215:VAL:HG13	2:B:294:ILE:HD13	1.97	0.47
2:B:563:ILE:HG22	2:B:595:LEU:CD2	2.44	0.47
2:B:563:ILE:HG22	2:B:595:LEU:HD23	1.97	0.46
1:A:329:MET:HB2	1:A:331:TYR:CE1	2.50	0.46
1:A:152:ASP:HB2	1:A:259:GLY:HA3	1.96	0.46
3:C:91:U:C2	4:D:39:A:N1	2.83	0.46
3:C:92:U:N3	4:D:38:A:C2	2.81	0.46
2:B:220:HIS:CE1	2:B:331:GLY:HA3	2.52	0.44
4:D:14:A:H1'	4:D:25:A:C6	2.52	0.44
2:B:332:PHE:CD1	2:B:378:LYS:HG2	2.52	0.44
1:A:317:VAL:HA	1:A:413:LEU:HA	1.99	0.44
1:A:160:THR:HG23	1:A:169:LEU:HD11	2.00	0.44
2:B:536:VAL:O	2:B:625:ALA:HA	2.18	0.43
4:D:37:C:C2	4:D:38:A:C8	3.06	0.43
4:D:24:A:C2	4:D:60:C:C2	3.06	0.43
4:D:82:C:H2'	4:D:83:G:C8	2.54	0.43
2:B:214:ASN:N	2:B:214:ASN:HD22	2.16	0.43
2:B:479:VAL:HG21	2:B:504:LEU:HD23	2.02	0.42
1:A:382:TYR:CG	1:A:389:LEU:HB2	2.56	0.41
2:B:207:ALA:HB1	2:B:208:PRO:HD2	2.03	0.41
1:A:317:VAL:HG12	1:A:413:LEU:HD23	2.03	0.41
1:A:157:LEU:HD12	1:A:171:LYS:HD2	2.03	0.41
1:A:43:ASP:CG	1:A:47:ARG:HH21	2.25	0.41
4:D:85:A:C2	4:D:86:C:C4	3.09	0.40
3:C:92:U:O2	3:C:93:G:C5	2.73	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 PDB entries followed by that with respect to all EM entries.

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	
1	A	412/414 (100%)	365 (89%)	34 (8%)	13 (3%)	5	41
2	B	426/428 (100%)	374 (88%)	37 (9%)	15 (4%)	4	39
All	All	838/842 (100%)	739 (88%)	71 (8%)	28 (3%)	8	40

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	145	LYS
1	A	326	LEU
2	B	298	PRO
2	B	315	ASP
1	A	43	ASP
1	A	144	SER
1	A	338	THR
2	B	277	THR
2	B	461	SER
2	B	543	ILE
2	B	564	THR
2	B	567	ILE
1	A	62	ILE
1	A	244	GLN
2	B	208	PRO
2	B	487	ASP
2	B	574	SER
1	A	64	SER
2	B	431	ASN
2	B	509	GLU
2	B	522	ASN
2	B	555	HIS
1	A	68	ARG
1	A	373	PRO

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Mol	Chain	Res	Type
2	B	475	ASN
1	A	63	LYS
1	A	190	PHE

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 PDB entries followed by that with respect to all EM entries.

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	
1	A	357/357 (100%)	342 (96%)	15 (4%)	36	70
2	B	372/372 (100%)	353 (95%)	19 (5%)	29	66
All	All	729/729 (100%)	695 (95%)	34 (5%)	37	68

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	PRO
1	A	42	LYS
1	A	51	MET
1	A	56	PHE
1	A	130	LYS
1	A	141	SER
1	A	201	TYR
1	A	208	THR
1	A	264	PHE
1	A	283	GLU
1	A	284	LYS
1	A	303	PHE
1	A	320	LEU
1	A	416	ARG
1	A	419	PHE
2	B	214	ASN
2	B	246	LYS
2	B	276	LYS
2	B	298	PRO
2	B	305	PRO

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Mol	Chain	Res	Type
2	B	343	MET
2	B	388	PHE
2	B	392	LYS
2	B	413	PHE
2	B	434	ARG
2	B	440	ILE
2	B	488	ASP
2	B	501	LYS
2	B	502	ILE
2	B	517	ILE
2	B	536	VAL
2	B	551	VAL
2	B	554	ILE
2	B	571	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	214	ASN
2	B	540	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	9/10 (90%)	6 (66%)	1 (11%)
4	D	87/88 (98%)	23 (26%)	6 (6%)
All	All	96/98 (97%)	29 (30%)	7 (7%)

All (29) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	91	U
3	C	92	U
3	C	94	U
3	C	96	A
3	C	97	A
3	C	99	A
4	D	7	G
4	D	8	U
4	D	10	G

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Mol	Chain	Res	Type
4	D	16	C
4	D	17	C
4	D	19	G
4	D	20	G
4	D	21	U
4	D	22	C
4	D	23	A
4	D	24	A
4	D	35	C
4	D	36	U
4	D	40	G
4	D	52	U
4	D	61	C
4	D	68	C
4	D	71	A
4	D	72	U
4	D	73	C
4	D	83	G
4	D	87	C
4	D	88	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	91	U
4	D	9	U
4	D	22	C
4	D	23	A
4	D	60	C
4	D	70	A
4	D	72	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.