



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 10:17 AM EST

PDB ID : 1GTS
Title : STRUCTURAL BASIS FOR TRANSFER RNA AMINOACYLATION BY
ESCHERICHIA COLI GLUTAMINYL-TRNA SYNTHETASE
Authors : Perona, J.J.; Steitz, T.A.; Rould, M.A.
Deposited on : 1993-09-15
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	rb-20028442

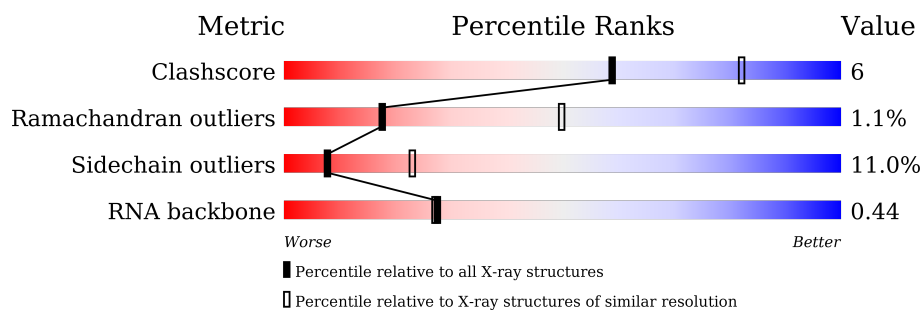
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	74	
2	A	553	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6004 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

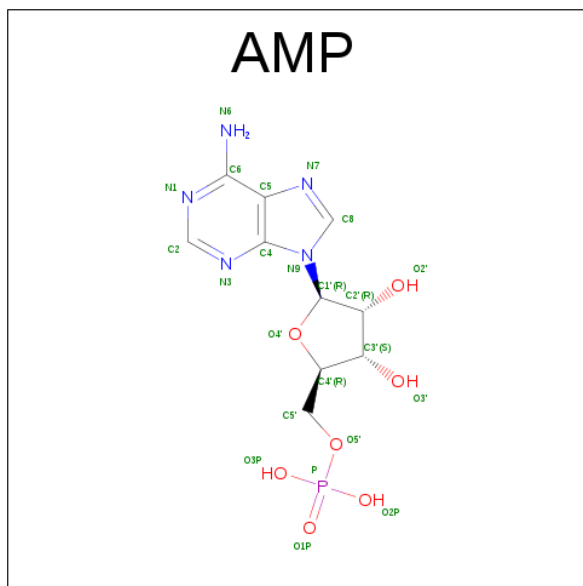
- Molecule 1 is a RNA chain called TRNAGLN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	74	Total	C	N	O	P	0	0	0
			1573	702	279	518	74			

- Molecule 2 is a protein called PROTEIN (GLUTAMINYL-TRNA SYNTHETASE (E.C.6.1.1.18)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	529	Total	C	N	O	S	0	0	0
			4279	2704	752	802	21			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is water.

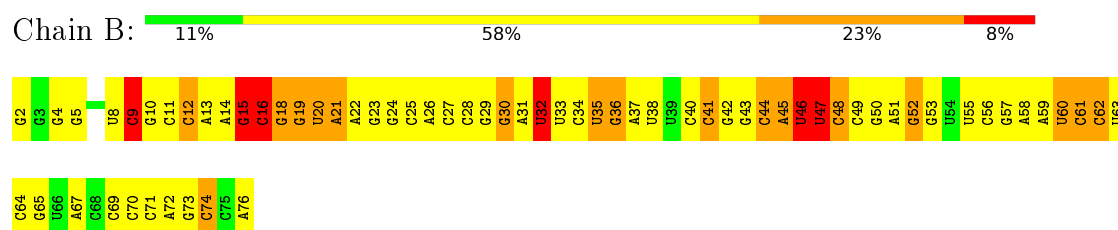
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total 112	O 112	0	0
4	B	17	Total 17	O 17	0	0

3 Residue-property plots

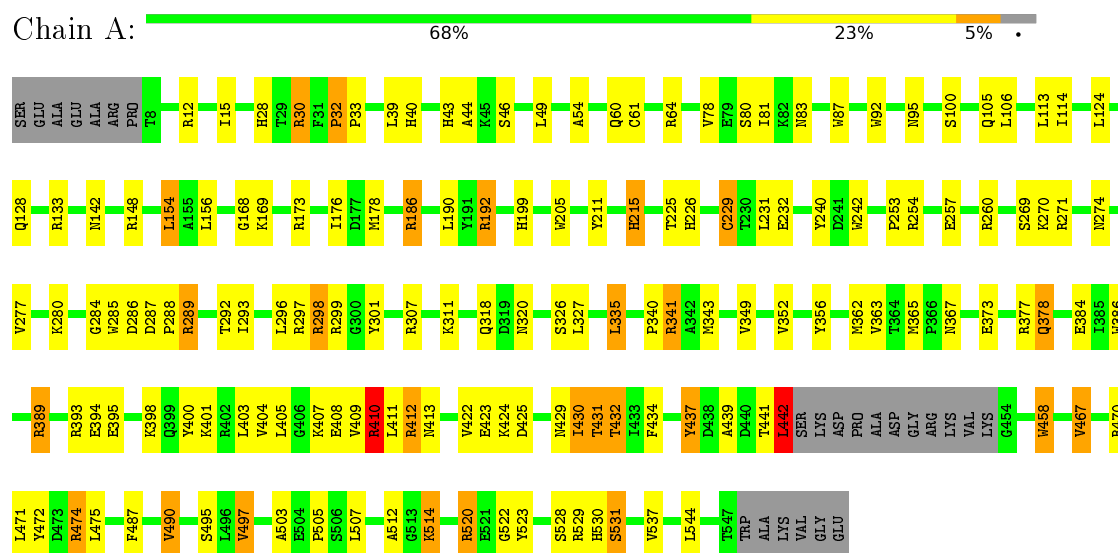
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: TRNAGLN



• Molecule 2: PROTEIN (GLUTAMINYL-TRNA SYNTHETASE (E.C.6.1.1.18))



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	242.84Å 93.59Å 115.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6004	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: AMP

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	B	1.31	1/1756 (0.1%)	3.14	198/2734 (7.2%)
2	A	0.78	0/4379	1.41	54/5928 (0.9%)
All	All	0.96	1/6135 (0.0%)	2.12	252/8662 (2.9%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	G	C4'-C3'	-5.15	1.47	1.52

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	G	O3'-P-O5'	34.02	168.65	104.00
1	B	31	A	OP2-P-O3'	27.85	166.48	105.20
1	B	15	G	OP1-P-O3'	23.01	155.82	105.20
1	B	32	U	OP1-P-O3'	-22.60	55.49	105.20
1	B	37	A	OP2-P-O3'	19.02	147.05	105.20
1	B	37	A	OP1-P-O3'	-18.93	63.56	105.20
1	B	46	U	OP2-P-O3'	-18.83	63.77	105.20
1	B	46	U	O3'-P-O5'	18.80	139.72	104.00
1	B	43	G	OP2-P-O3'	-18.17	65.23	105.20
1	B	47	U	O3'-P-O5'	-17.51	70.73	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	A	OP1-P-O3'	-17.25	67.26	105.20
1	B	61	C	OP1-P-O3'	-17.09	67.60	105.20
1	B	19	G	OP1-P-O3'	16.98	142.55	105.20
1	B	15	G	O3'-P-O5'	-16.96	71.78	104.00
1	B	51	A	OP2-P-O3'	16.72	141.99	105.20
1	B	40	C	OP2-P-O3'	16.67	141.88	105.20
1	B	63	U	OP2-P-O3'	15.66	139.65	105.20
1	B	16	C	OP2-P-O3'	15.64	139.61	105.20
1	B	20	U	OP1-P-O3'	-15.40	71.31	105.20
1	B	40	C	O3'-P-O5'	-15.38	74.78	104.00
1	B	47	U	OP2-P-O3'	15.25	138.75	105.20
1	B	13	A	O3'-P-O5'	15.16	132.81	104.00
1	B	21	A	OP1-P-O3'	-15.08	72.03	105.20
1	B	34	C	OP1-P-O3'	15.07	138.36	105.20
1	B	31	A	O3'-P-O5'	-14.64	76.18	104.00
1	B	51	A	OP1-P-O3'	-14.62	73.04	105.20
1	B	4	G	OP2-P-O3'	14.03	136.06	105.20
1	B	14	A	O3'-P-O5'	13.83	130.28	104.00
1	B	19	G	OP2-P-O3'	-13.64	75.20	105.20
1	B	32	U	O3'-P-O5'	12.82	128.35	104.00
1	B	50	G	OP1-P-O3'	-12.63	77.42	105.20
1	B	61	C	O3'-P-O5'	12.31	127.40	104.00
1	B	58	A	OP1-P-O3'	12.24	132.14	105.20
1	B	29	G	OP2-P-O3'	12.15	131.94	105.20
1	B	16	C	OP1-P-O3'	-11.97	78.87	105.20
1	B	21	A	OP2-P-O3'	11.80	131.17	105.20
1	B	45	A	OP1-P-O3'	11.78	131.12	105.20
1	B	52	G	OP1-P-O3'	-11.68	79.51	105.20
1	B	32	U	O4'-C1'-N1	11.53	117.42	108.20
1	B	28	C	O3'-P-O5'	11.52	125.88	104.00
1	B	13	A	OP1-P-O3'	-11.29	80.36	105.20
1	B	26	A	OP1-P-O3'	-11.09	80.79	105.20
1	B	55	U	OP2-P-O3'	10.84	129.06	105.20
1	B	9	C	OP2-P-O3'	10.80	128.96	105.20
1	B	67	A	OP1-P-O3'	10.79	128.94	105.20
1	B	15	G	OP2-P-O3'	-10.77	81.51	105.20
1	B	71	C	O3'-P-O5'	10.59	124.11	104.00
1	B	29	G	OP1-P-O3'	-10.57	81.94	105.20
1	B	49	C	OP2-P-O3'	10.45	128.20	105.20
1	B	63	U	OP1-P-O3'	-10.42	82.28	105.20
1	B	60	U	OP2-P-O3'	10.31	127.89	105.20
1	B	49	C	OP1-P-O3'	-10.17	82.83	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	C	OP1-P-O3'	-9.87	83.49	105.20
1	B	27	C	O3'-P-O5'	9.85	122.71	104.00
1	B	44	C	O3'-P-O5'	-9.84	85.30	104.00
1	B	30	G	O4'-C1'-N9	9.75	116.00	108.20
1	B	64	C	O3'-P-O5'	-9.69	85.59	104.00
1	B	52	G	O3'-P-O5'	9.62	122.27	104.00
1	B	4	G	OP1-P-O3'	-9.59	84.10	105.20
1	B	15	G	O4'-C1'-N9	9.43	115.75	108.20
1	B	28	C	OP1-P-O3'	-9.39	84.54	105.20
1	B	43	G	OP1-P-O3'	-9.19	84.99	105.20
1	B	18	G	O3'-P-O5'	-9.03	86.84	104.00
1	B	20	U	O3'-P-O5'	9.03	121.15	104.00
1	B	27	C	OP1-P-O3'	-8.85	85.73	105.20
1	B	5	G	OP1-P-O3'	8.84	124.66	105.20
1	B	20	U	OP2-P-O3'	8.71	124.37	105.20
2	A	12	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	72	A	OP2-P-O3'	8.54	123.98	105.20
1	B	69	C	OP1-P-O3'	8.41	123.71	105.20
1	B	2	G	OP1-P-O3'	-8.34	86.85	105.20
2	A	260	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	B	4	G	O4'-C1'-N9	8.27	114.81	108.20
1	B	50	G	OP2-P-O3'	8.26	123.36	105.20
2	A	173	ARG	NE-CZ-NH2	-8.25	116.18	120.30
2	A	205	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	B	28	C	N1-C2-O2	8.22	123.83	118.90
1	B	31	A	O4'-C1'-N9	8.20	114.76	108.20
2	A	92	TRP	CD1-CG-CD2	8.20	112.86	106.30
1	B	30	G	C1'-O4'-C4'	-8.13	103.39	109.90
1	B	8	U	O3'-P-O5'	8.12	119.42	104.00
2	A	386	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	B	32	U	N1-C1'-C2'	-8.09	103.10	112.00
1	B	34	C	O3'-P-O5'	-8.05	88.70	104.00
2	A	458	TRP	CD1-CG-CD2	8.02	112.72	106.30
1	B	42	G	O4'-C1'-N9	7.97	114.57	108.20
2	A	285	TRP	CD1-CG-CD2	7.94	112.66	106.30
2	A	242	TRP	CD1-CG-CD2	7.89	112.61	106.30
1	B	40	C	N1-C2-O2	7.86	123.61	118.90
1	B	14	A	OP1-P-O3'	-7.85	87.93	105.20
1	B	2	G	OP2-P-O3'	7.82	122.40	105.20
1	B	11	C	OP1-P-O3'	-7.81	88.03	105.20
1	B	46	U	O4'-C1'-N1	7.80	114.44	108.20
2	A	298	ARG	NE-CZ-NH1	7.77	124.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	205	TRP	CE2-CD2-CG	-7.73	101.11	107.30
1	B	72	A	O3'-P-O5'	-7.72	89.32	104.00
1	B	46	U	C1'-O4'-C4'	-7.71	103.74	109.90
2	A	148	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	B	71	C	N1-C2-O2	7.69	123.51	118.90
2	A	173	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	B	34	C	N1-C2-O2	7.63	123.48	118.90
2	A	285	TRP	CE2-CD2-CG	-7.61	101.22	107.30
1	B	44	C	N1-C2-O2	7.60	123.46	118.90
1	B	41	C	N1-C2-O2	7.52	123.41	118.90
2	A	87	TRP	CD1-CG-CD2	7.46	112.27	106.30
2	A	520	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	B	53	G	O3'-P-O5'	7.45	118.15	104.00
1	B	9	C	OP1-P-O3'	-7.44	88.84	105.20
1	B	62	C	N1-C2-O2	7.42	123.35	118.90
1	B	11	C	O3'-P-O5'	7.39	118.04	104.00
1	B	70	C	N1-C2-O2	7.38	123.33	118.90
1	B	69	C	N1-C2-O2	7.37	123.32	118.90
2	A	458	TRP	CE2-CD2-CG	-7.36	101.41	107.30
2	A	242	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	B	70	C	O3'-P-O5'	-7.33	90.08	104.00
1	B	55	U	OP1-P-O3'	-7.32	89.10	105.20
1	B	23	G	O3'-P-O5'	7.30	117.88	104.00
1	B	35	U	OP2-P-O3'	7.26	121.18	105.20
1	B	70	C	O4'-C1'-N1	7.25	114.00	108.20
1	B	45	A	P-O3'-C3'	7.23	128.38	119.70
2	A	341	ARG	NE-CZ-NH1	7.16	123.88	120.30
2	A	386	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	B	62	C	O3'-P-O5'	7.11	117.51	104.00
1	B	45	A	OP2-P-O3'	-7.08	89.63	105.20
1	B	32	U	OP2-P-O3'	7.01	120.63	105.20
2	A	92	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	B	73	G	O3'-P-O5'	-6.98	90.73	104.00
1	B	41	C	O4'-C1'-N1	6.95	113.76	108.20
1	B	74	C	O3'-P-O5'	-6.94	90.81	104.00
2	A	242	TRP	CG-CD2-CE3	6.93	140.14	133.90
1	B	65	G	O3'-P-O5'	-6.90	90.90	104.00
1	B	34	C	OP2-P-O3'	-6.89	90.04	105.20
1	B	46	U	C5'-C4'-O4'	6.89	117.37	109.10
1	B	61	C	OP2-P-O3'	6.87	120.32	105.20
2	A	299	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	A	148	ARG	NE-CZ-NH2	-6.67	116.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	C	P-O3'-C3'	6.67	127.70	119.70
1	B	15	G	P-O3'-C3'	6.66	127.69	119.70
2	A	87	TRP	CE2-CD2-CG	-6.66	101.98	107.30
1	B	71	C	OP1-P-O3'	-6.63	90.62	105.20
1	B	30	G	N9-C1'-C2'	-6.58	104.76	112.00
1	B	34	C	O4'-C1'-C2'	-6.57	99.23	105.80
1	B	48	C	N1-C2-O2	6.57	122.84	118.90
1	B	40	C	OP1-P-O3'	-6.53	90.84	105.20
2	A	412	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	56	C	N1-C2-O2	6.45	122.77	118.90
2	A	242	TRP	CB-CG-CD1	-6.44	118.63	127.00
2	A	297	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	53	G	OP1-P-O3'	-6.43	91.05	105.20
1	B	74	C	OP1-P-O3'	6.42	119.33	105.20
2	A	410	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	15	G	N9-C1'-C2'	-6.41	104.95	112.00
1	B	70	C	N3-C2-O2	-6.32	117.48	121.90
1	B	8	U	N3-C4-C5	-6.32	110.81	114.60
1	B	61	C	N1-C2-O2	6.28	122.67	118.90
2	A	298	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	B	40	C	N3-C2-O2	-6.24	117.53	121.90
1	B	28	C	N3-C2-O2	-6.20	117.56	121.90
1	B	12	C	C4'-C3'-C2'	-6.19	96.41	102.60
1	B	64	C	N1-C2-O2	6.19	122.61	118.90
1	B	74	C	P-O3'-C3'	6.18	127.11	119.70
1	B	47	U	O4'-C1'-C2'	-6.15	99.65	105.80
1	B	45	A	C1'-O4'-C4'	-6.14	104.99	109.90
2	A	520	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	9	C	O4'-C1'-N1	6.12	113.10	108.20
1	B	26	A	O4'-C4'-C3'	-6.11	97.89	104.00
1	B	22	A	O4'-C1'-N9	6.10	113.08	108.20
1	B	63	U	O3'-P-O5'	-6.02	92.56	104.00
1	B	16	C	N1-C2-O2	5.98	122.49	118.90
1	B	64	C	O4'-C1'-N1	5.92	112.94	108.20
1	B	43	G	O4'-C1'-N9	5.91	112.92	108.20
1	B	37	A	O4'-C1'-N9	5.89	112.91	108.20
1	B	18	G	OP1-P-O3'	5.88	118.14	105.20
1	B	47	U	C1'-O4'-C4'	-5.87	105.21	109.90
2	A	87	TRP	CG-CD2-CE3	5.83	139.14	133.90
2	A	133	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	14	A	C1'-O4'-C4'	-5.81	105.25	109.90
2	A	12	ARG	NE-CZ-NH1	5.81	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	A	P-O3'-C3'	-5.79	112.75	119.70
1	B	20	U	P-O3'-C3'	5.75	126.60	119.70
1	B	32	U	C5'-C4'-O4'	5.75	116.00	109.10
1	B	32	U	P-O5'-C5'	5.74	130.09	120.90
1	B	38	U	O3'-P-O5'	5.74	114.91	104.00
2	A	343	MET	CG-SD-CE	-5.72	91.05	100.20
2	A	467	VAL	CA-CB-CG2	-5.71	102.33	110.90
1	B	35	U	OP1-P-O3'	-5.71	92.64	105.20
1	B	63	U	C5'-C4'-C3'	-5.64	106.97	116.00
1	B	41	C	P-O5'-C5'	5.63	129.91	120.90
2	A	297	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	A	289	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	60	U	C5'-C4'-C3'	-5.59	107.06	116.00
1	B	29	G	C5'-C4'-C3'	-5.59	107.06	116.00
1	B	22	A	C5'-C4'-C3'	-5.58	107.07	116.00
1	B	11	C	P-O3'-C3'	-5.56	113.03	119.70
1	B	10	G	P-O3'-C3'	-5.56	113.03	119.70
2	A	307	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	A	64	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	28	C	O4'-C1'-N1	5.54	112.64	108.20
1	B	41	C	N3-C2-O2	-5.51	118.05	121.90
1	B	32	U	O4'-C4'-C3'	-5.47	98.53	104.00
2	A	87	TRP	CG-CD1-NE1	-5.46	104.64	110.10
2	A	173	ARG	CB-CG-CD	-5.43	97.48	111.60
2	A	242	TRP	CG-CD1-NE1	-5.42	104.68	110.10
1	B	76	A	O4'-C1'-N9	5.41	112.53	108.20
1	B	25	C	O3'-P-O5'	5.40	114.26	104.00
1	B	52	G	C5'-C4'-C3'	-5.40	107.37	116.00
1	B	31	A	N9-C1'-C2'	-5.39	106.07	112.00
1	B	34	C	N3-C2-O2	-5.36	118.15	121.90
2	A	458	TRP	CG-CD1-NE1	-5.36	104.75	110.10
1	B	64	C	OP2-P-O3'	5.35	116.98	105.20
1	B	72	A	P-O3'-C3'	5.34	126.11	119.70
2	A	442	LEU	CA-CB-CG	5.34	127.59	115.30
1	B	40	C	O4'-C1'-N1	5.30	112.44	108.20
1	B	59	A	N1-C6-N6	5.29	121.77	118.60
1	B	38	U	C5'-C4'-C3'	-5.28	107.55	116.00
2	A	215	HIS	CA-CB-CG	-5.25	104.68	113.60
1	B	33	U	O4'-C1'-N1	5.25	112.40	108.20
2	A	472	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	B	48	C	P-O5'-C5'	5.24	129.28	120.90
1	B	63	U	N3-C2-O2	-5.24	118.53	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	C	O3'-P-O5'	-5.24	94.05	104.00
1	B	32	U	C1'-O4'-C4'	-5.23	105.71	109.90
2	A	205	TRP	CG-CD1-NE1	-5.23	104.87	110.10
2	A	280	LYS	CA-CB-CG	5.21	124.86	113.40
1	B	27	C	N1-C2-O2	5.21	122.02	118.90
1	B	19	G	O3'-P-O5'	-5.21	94.11	104.00
1	B	30	G	O4'-C4'-C3'	-5.19	98.81	104.00
1	B	67	A	O3'-P-O5'	-5.18	94.16	104.00
1	B	44	C	N3-C2-O2	-5.16	118.29	121.90
2	A	474	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	26	A	O3'-P-O5'	5.16	113.80	104.00
1	B	57	G	O3'-P-O5'	-5.16	94.20	104.00
1	B	24	G	O4'-C1'-N9	5.14	112.31	108.20
1	B	56	C	N3-C2-O2	-5.14	118.30	121.90
1	B	11	C	C3'-C2'-C1'	-5.12	97.40	101.50
2	A	356	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	B	73	G	O4'-C1'-N9	5.11	112.29	108.20
1	B	30	G	C4'-C3'-C2'	-5.11	97.49	102.60
2	A	92	TRP	CG-CD1-NE1	-5.11	105.00	110.10
1	B	5	G	O3'-P-O5'	-5.09	94.33	104.00
2	A	192	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	26	A	P-O3'-C3'	-5.08	113.61	119.70
1	B	41	C	C5'-C4'-O4'	5.06	115.17	109.10
1	B	26	A	OP2-P-O3'	5.06	116.33	105.20
1	B	60	U	P-O3'-C3'	-5.05	113.64	119.70
1	B	69	C	N3-C2-O2	-5.05	118.36	121.90
1	B	38	U	OP2-P-O3'	-5.04	94.12	105.20
1	B	70	C	OP2-P-O3'	5.03	116.26	105.20
2	A	470	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	12	C	N1-C2-O2	5.01	121.91	118.90
1	B	4	G	P-O3'-C3'	-5.00	113.69	119.70
1	B	42	G	C1'-O4'-C4'	-5.00	105.90	109.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	211	TYR	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	B	1573	0	800	11	0
2	A	4279	0	4172	55	0
3	A	23	0	12	0	0
4	A	112	0	0	0	0
4	B	17	0	0	0	0
All	All	6004	0	4984	62	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 6.

All (62) 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)
2:A:39:LEU:HD13	2:A:81:ILE:HG12	1.62	0.81
2:A:424:LYS:HA	2:A:430:ILE:HA	1.63	0.79
2:A:403:LEU:HD13	2:A:409:VAL:HG22	1.71	0.73
2:A:44:ALA:HB2	2:A:293:ILE:HD11	1.72	0.71
2:A:352:VAL:HG12	2:A:384:GLU:HG2	1.71	0.71
2:A:363:VAL:HG11	2:A:413:ASN:O	1.92	0.69
2:A:40:HIS:HA	2:A:292:THR:HA	1.81	0.63
1:B:46:U:H4'	1:B:47:U:C5	2.34	0.62
2:A:114:ILE:HG21	2:A:154:LEU:HD13	1.83	0.58
1:B:12:C:H5''	2:A:320:ASN:HB2	1.86	0.58
2:A:393:ARG:O	2:A:404:VAL:HA	2.04	0.57
2:A:287:ASP:OD1	2:A:289:ARG:HD3	2.05	0.57
1:B:60:U:H5''	1:B:61:C:H5	1.69	0.56
2:A:277:VAL:HG13	2:A:284:GLY:HA2	1.91	0.53
2:A:43:HIS:HE1	2:A:270:LYS:HE2	1.73	0.52
2:A:425:ASP:HB2	2:A:431:THR:HG23	1.90	0.52
2:A:471:LEU:HB2	2:A:497:VAL:HG13	1.91	0.51
1:B:32:U:OP2	1:B:32:U:H3'	2.11	0.51
2:A:114:ILE:CG2	2:A:154:LEU:HD13	2.40	0.51
2:A:30:ARG:NH1	2:A:215:HIS:CE1	2.79	0.50
2:A:288:PRO:HG3	2:A:298:ARG:HG2	1.93	0.50
2:A:487:PHE:O	2:A:490:VAL:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:C:N3	2:A:168:GLY:HA2	2.26	0.50
2:A:240:TYR:OH	2:A:253:PRO:HB2	2.12	0.49
2:A:225:THR:OG1	2:A:226:HIS:HD2	1.94	0.49
2:A:335:LEU:HB3	2:A:523:TYR:CD2	2.48	0.48
2:A:424:LYS:HG2	2:A:430:ILE:HG13	1.94	0.48
2:A:229:CYS:O	2:A:257:GLU:HA	2.13	0.48
2:A:340:PRO:HG3	2:A:514:LYS:HE2	1.96	0.47
2:A:437:TYR:CE2	2:A:439:ALA:HA	2.49	0.47
2:A:286:ASP:O	2:A:298:ARG:HD3	2.16	0.46
1:B:9:C:H5	1:B:12:C:N4	2.12	0.46
2:A:80:SER:O	2:A:83:ASN:HB3	2.16	0.46
2:A:296:LEU:O	2:A:301:TYR:HB2	2.17	0.45
2:A:411:LEU:HB3	2:A:458:TRP:CD1	2.52	0.45
2:A:349:VAL:HB	2:A:389:ARG:HD3	1.99	0.44
2:A:367:ASN:OD1	2:A:377:ARG:HD3	2.17	0.44
1:B:35:U:H1'	2:A:520:ARG:HG2	2.00	0.44
2:A:124:LEU:HG	2:A:128:GLN:HB3	2.00	0.44
2:A:512:ALA:HB2	2:A:528:SER:OG	2.18	0.43
2:A:394:GLU:HG2	2:A:405:LEU:HD22	2.00	0.43
1:B:36:G:C6	2:A:401:LYS:HG2	2.53	0.43
2:A:425:ASP:HB3	2:A:429:ASN:HB2	1.99	0.43
2:A:423:GLU:HB2	2:A:434:PHE:HE1	1.82	0.43
2:A:178:MET:O	2:A:186:ARG:HD2	2.19	0.43
2:A:28:HIS:CD2	2:A:60:GLN:HB2	2.54	0.43
2:A:530:HIS:HB3	2:A:537:VAL:HG21	1.99	0.43
2:A:142:ASN:HD22	2:A:178:MET:HG3	1.84	0.43
2:A:531:SER:HB3	2:A:537:VAL:H	1.83	0.42
1:B:15:G:O2'	1:B:16:C:P	2.77	0.42
1:B:46:U:OP1	1:B:47:U:H5'	2.19	0.42
2:A:362:MET:HG2	2:A:378:GLN:HG3	2.01	0.42
1:B:46:U:H6	1:B:46:U:H2'	1.68	0.41
2:A:423:GLU:HB3	2:A:432:THR:HG23	2.01	0.41
2:A:503:ALA:HB1	2:A:507:LEU:CD2	2.50	0.41
2:A:407:LYS:HG2	2:A:408:GLU:H	1.85	0.41
2:A:410:ARG:HH21	2:A:442:LEU:HA	1.85	0.41
2:A:522:GLY:HA2	2:A:544:LEU:HD13	2.02	0.41
2:A:393:ARG:HB2	2:A:400:TYR:CZ	2.55	0.41
2:A:254:ARG:HD3	2:A:254:ARG:HA	1.86	0.40
2:A:54:ALA:HB2	2:A:61:CYS:HB2	2.02	0.40
2:A:15:ILE:HG12	2:A:226:HIS:CE1	2.57	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	A	525/553 (95%)	490 (93%)	29 (6%)	6 (1%)	17	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	32	PRO
2	A	199	HIS
2	A	398	LYS
2	A	430	ILE
2	A	529	ARG
2	A	176	ILE

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	463/481 (96%)	412 (89%)	51 (11%)	8	23

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	30	ARG
2	A	32	PRO
2	A	33	PRO
2	A	46	SER
2	A	49	LEU

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Mol	Chain	Res	Type
2	A	78	VAL
2	A	95	ASN
2	A	100	SER
2	A	105	GLN
2	A	106	LEU
2	A	113	LEU
2	A	154	LEU
2	A	156	LEU
2	A	169	LYS
2	A	186	ARG
2	A	190	LEU
2	A	192	ARG
2	A	229	CYS
2	A	231	LEU
2	A	232	GLU
2	A	269	SER
2	A	271	ARG
2	A	274	ASN
2	A	311	LYS
2	A	318	GLN
2	A	326	SER
2	A	327	LEU
2	A	335	LEU
2	A	341	ARG
2	A	365	MET
2	A	373	GLU
2	A	378	GLN
2	A	389	ARG
2	A	395	GLU
2	A	410	ARG
2	A	412	ARG
2	A	422	VAL
2	A	431	THR
2	A	432	THR
2	A	437	TYR
2	A	441	THR
2	A	442	LEU
2	A	467	VAL
2	A	474	ARG
2	A	475	LEU
2	A	490	VAL
2	A	495	SER

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Mol	Chain	Res	Type
2	A	497	VAL
2	A	505	PRO
2	A	514	LYS
2	A	531	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	60	GLN
2	A	142	ASN
2	A	226	HIS
2	A	274	ASN
2	A	355	ASN
2	A	413	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	73/74 (98%)	16 (21%)	6 (8%)

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	9	C
1	B	16	C
1	B	18	G
1	B	19	G
1	B	20	U
1	B	21	A
1	B	30	G
1	B	32	U
1	B	41	C
1	B	44	C
1	B	45	A
1	B	46	U
1	B	47	U
1	B	48	C
1	B	52	G
1	B	62	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	15	G
1	B	16	C
1	B	20	U
1	B	36	G
1	B	44	C
1	B	45	A

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](#)

1 ligand is 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	$\# Z > 2$
3	AMP	A	999	-	22,25,25	1.09	1 (4%)	22,38,38	1.06	1 (4%)

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
3	AMP	A	999	-	-	0/6/26/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	AMP	P-O2P	-2.16	1.47	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	999	AMP	O2P-P-O1P	2.07	117.39	110.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.