



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 06:51 am BST

PDB ID : 1EFW  
Title : Crystal structure of aspartyl-tRNA synthetase from *Thermus thermophilus* complexed to tRNA<sup>asp</sup> from *Escherichia coli*  
Authors : Briand, C.; Poterszman, A.; Eiler, S.; Webster, G.; Thierry, J.-C.; Moras, D.  
Deposited on : 2000-02-10  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

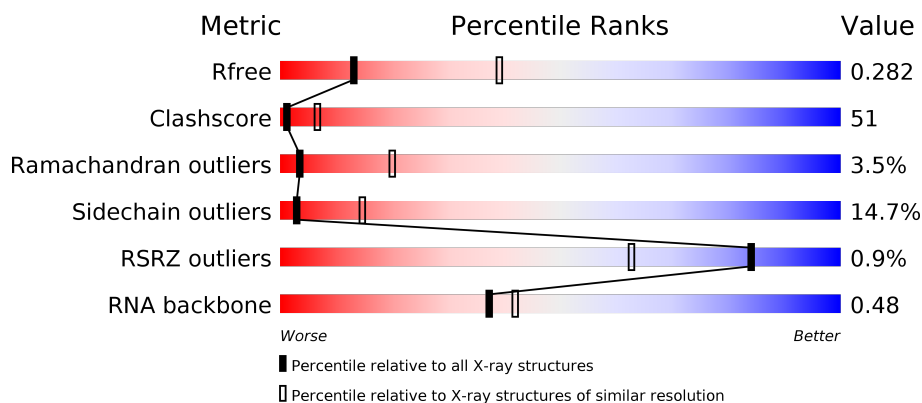
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


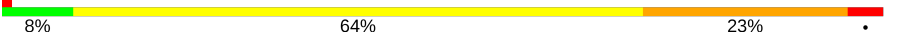


The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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

Mol	Chain	Length	Quality of chain
1	C	73	
1	D	73	
2	A	580	
2	B	580	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12572 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 ASPARTYL-TRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	73	Total	C	N	O	P	S	0	0	0
			1570	703	274	519	73	1			
1	D	73	Total	C	N	O	P	S	0	0	0
			1570	703	274	519	73	1			

- Molecule 2 is a protein called ASPARTYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	580	Total	C	N	O	S	0	0	0
			4668	2980	840	837	11			
2	B	580	Total	C	N	O	S	0	0	0
			4668	2980	840	837	11			

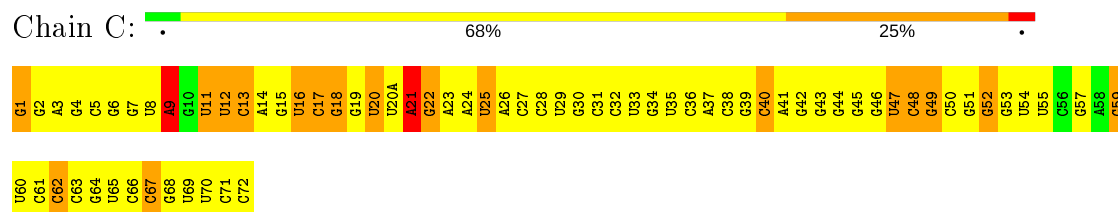
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	12	Total	O	0	0
			12	12		
3	D	10	Total	O	0	0
			10	10		
3	A	43	Total	O	0	0
			43	43		
3	B	31	Total	O	0	0
			31	31		

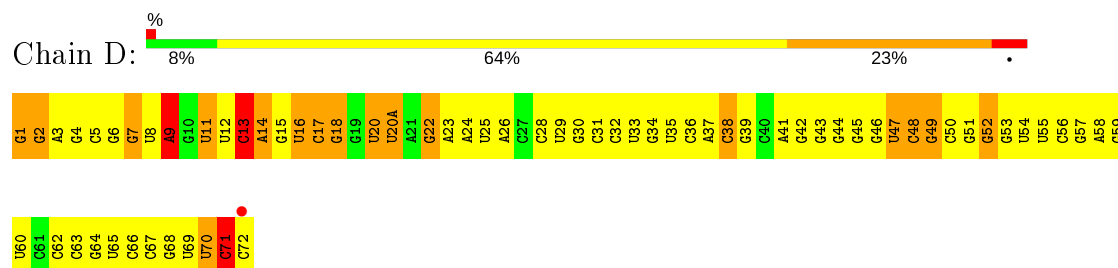
### 3 Residue-property plots

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

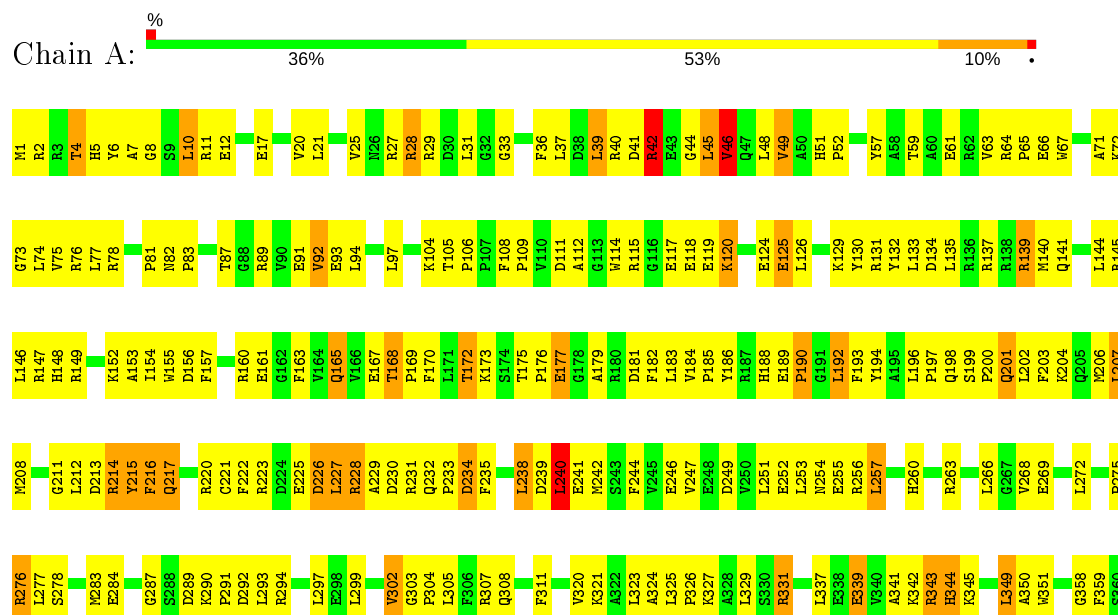
#### • Molecule 1: ASPARTYL-TRNA

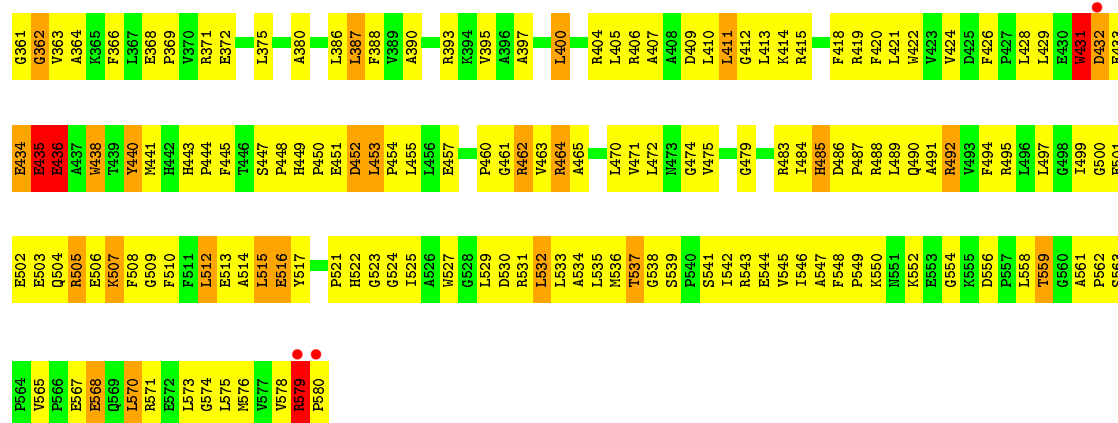


#### • Molecule 1: ASPARTYL-TRNA



#### • Molecule 2: ASPARTYL-TRNA SYNTHETASE





## • Molecule 2: ASPARTYL-TRNA SYNTHETASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	251.45Å 251.45Å 88.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.00 14.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.8 (15.00-3.00) 91.8 (14.99-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.87 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.248 , 0.293 0.238 , 0.282	Depositor DCC
$R_{free}$ test set	2969 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 16.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	12572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, G7M, H2U, 2MA, 4SU, QUO, 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	C	0.98	6/1506 (0.4%)	1.08	10/2343 (0.4%)
1	D	0.74	1/1506 (0.1%)	0.98	8/2343 (0.3%)
2	A	0.55	2/4780 (0.0%)	1.01	16/6467 (0.2%)
2	B	0.59	6/4780 (0.1%)	1.03	18/6467 (0.3%)
All	All	0.65	15/12572 (0.1%)	1.02	52/17620 (0.3%)

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	C	0	4
1	D	0	4
All	All	0	8

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	580	PRO	C-OXT	15.85	1.53	1.23
1	C	1	G	O3'-P	-15.47	1.42	1.61
1	C	59	G	O3'-P	12.60	1.76	1.61
2	A	495	ARG	CZ-NH1	11.61	1.48	1.33
2	A	495	ARG	CZ-NH2	10.79	1.47	1.33

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	307	ARG	NE-CZ-NH1	35.08	137.84	120.30
2	A	495	ARG	NE-CZ-NH2	-31.89	104.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	495	ARG	NH1-CZ-NH2	19.00	140.31	119.40
2	B	307	ARG	NE-CZ-NH2	-17.90	111.35	120.30
2	B	307	ARG	CG-CD-NE	17.16	147.83	111.80

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	21	A	Sidechain
1	C	25	U	Sidechain
1	C	40	C	Sidechain
1	C	9	A	Sidechain
1	D	7	G	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	C	1570	0	807	111	0
1	D	1570	0	805	132	0
2	A	4668	0	4679	469	0
2	B	4668	0	4679	548	0
3	A	43	0	0	3	0
3	B	31	0	0	7	0
3	C	12	0	0	1	0
3	D	10	0	0	0	0
All	All	12572	0	10970	1183	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 51.

The worst 5 of 1183 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)
1:D:2:G:H1	1:D:71:C:N4	1.40	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:ARG:HH21	2:B:29:ARG:NH1	1.42	1.17
1:D:37:2MA:H5''	2:B:27:ARG:HH12	1.01	1.11
1:D:68:G:H2'	1:D:69:U:C6	1.88	1.08
1:D:34:QUO:H4'	1:D:35:U:H5'	1.35	1.08

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	578/580 (100%)	499 (86%)	64 (11%)	15 (3%)	5	27
2	B	578/580 (100%)	459 (79%)	93 (16%)	26 (4%)	2	14
All	All	1156/1160 (100%)	958 (83%)	157 (14%)	41 (4%)	3	20

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	188	HIS
2	A	462	ARG
2	A	579	ARG
2	B	42	ARG
2	B	227	LEU

### 5.3.2 Protein sidechains [i](#)

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	483/483 (100%)	410 (85%)	73 (15%)	3	14
2	B	483/483 (100%)	414 (86%)	69 (14%)	3	15
All	All	966/966 (100%)	824 (85%)	142 (15%)	3	15

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	507	LYS
2	B	39	LEU
2	B	462	ARG
2	A	516	GLU
2	A	579	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	308	GLN
2	A	443	HIS
2	B	260	HIS
2	A	254	ASN
2	B	237	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	70/73 (95%)	9 (12%)	3 (4%)
1	D	70/73 (95%)	13 (18%)	3 (4%)
All	All	140/146 (95%)	22 (15%)	6 (4%)

5 of 22 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	9	A
1	C	16	H2U
1	C	17	C
1	C	18	G
1	C	20	H2U

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	48	C
1	D	48	C
1	D	17	C
1	C	47	U
1	D	47	U

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

20 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
1	H2U	C	20(A)	1	18,21,22	0.53	0	21,30,33	0.79	0
1	4SU	D	8	1	14,21,22	6.17	2 (14%)	15,30,33	2.84	2 (13%)
1	H2U	C	20	1	18,21,22	0.90	1 (5%)	21,30,33	0.71	0
1	QUO	C	34	1	28,35,36	1.36	5 (17%)	32,52,55	4.03	12 (37%)
1	5MU	D	54	1	15,22,23	1.92	4 (26%)	16,32,35	11.08	4 (25%)
1	G7M	D	46	1	20,26,27	1.19	2 (10%)	20,39,42	2.72	6 (30%)
1	PSU	C	65	1	17,21,22	2.25	4 (23%)	20,30,33	5.77	5 (25%)
1	PSU	D	65	1	17,21,22	1.94	4 (23%)	20,30,33	5.68	5 (25%)
1	G7M	C	46	1	20,26,27	1.22	2 (10%)	20,39,42	2.62	5 (25%)
1	QUO	D	34	1	28,35,36	1.22	3 (10%)	32,52,55	3.94	12 (37%)
1	H2U	D	16	1	18,21,22	0.66	1 (5%)	21,30,33	0.81	0
1	5MU	C	54	1	15,22,23	1.17	2 (13%)	16,32,35	3.69	2 (12%)
1	2MA	C	37	1	17,25,26	0.75	1 (5%)	19,37,40	2.01	2 (10%)
1	PSU	D	55	1	17,21,22	1.94	4 (23%)	20,30,33	5.76	5 (25%)
1	H2U	C	16	1	18,21,22	0.93	1 (5%)	21,30,33	0.82	1 (4%)
1	H2U	D	20(A)	1	18,21,22	0.81	1 (5%)	21,30,33	0.82	0
1	H2U	D	20	1	18,21,22	0.70	1 (5%)	21,30,33	0.83	1 (4%)
1	4SU	C	8	1	14,21,22	6.10	2 (14%)	15,30,33	2.86	2 (13%)
1	PSU	C	55	1	17,21,22	1.99	4 (23%)	20,30,33	5.80	5 (25%)
1	2MA	D	37	1	17,25,26	0.64	0	19,37,40	2.04	2 (10%)

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
1	H2U	C	20(A)	1	-	1/7/38/39	0/2/2/2
1	4SU	D	8	1	-	0/5/25/26	0/2/2/2
1	H2U	C	20	1	-	0/7/38/39	0/2/2/2
1	QUO	C	34	1	-	2/6/43/44	0/4/4/4
1	5MU	D	54	1	-	0/5/25/26	0/2/2/2
1	G7M	D	46	1	-	0/3/25/26	0/3/3/3
1	PSU	C	65	1	-	0/7/25/26	0/2/2/2
1	PSU	D	65	1	-	0/7/25/26	0/2/2/2
1	G7M	C	46	1	-	0/3/25/26	0/3/3/3
1	QUO	D	34	1	-	1/6/43/44	0/4/4/4
1	H2U	D	16	1	-	2/7/38/39	0/2/2/2
1	5MU	C	54	1	-	0/5/25/26	0/2/2/2
1	2MA	C	37	1	-	1/3/25/26	0/3/3/3
1	PSU	D	55	1	-	1/7/25/26	0/2/2/2
1	H2U	C	16	1	-	2/7/38/39	0/2/2/2
1	H2U	D	20(A)	1	-	3/7/38/39	0/2/2/2
1	H2U	D	20	1	-	7/7/38/39	0/2/2/2
1	4SU	C	8	1	-	1/5/25/26	0/2/2/2
1	PSU	C	55	1	-	0/7/25/26	0/2/2/2
1	2MA	D	37	1	-	1/3/25/26	0/3/3/3

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	8	4SU	C4-S4	-22.45	1.26	1.67
1	C	8	4SU	C4-S4	-22.17	1.26	1.67
1	C	65	PSU	C5-C1'	-6.42	1.46	1.52
1	C	55	PSU	C5-C1'	-5.07	1.47	1.52
1	C	65	PSU	C6-N1	-4.96	1.23	1.34

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54	5MU	C5M-C5-C4	-42.38	45.44	121.37
1	D	55	PSU	N1-C2-N3	-17.60	114.44	128.43
1	C	65	PSU	N1-C2-N3	-17.41	114.59	128.43
1	C	55	PSU	N1-C2-N3	-17.35	114.63	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	PSU	N1-C2-N3	-17.18	114.77	128.43

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	34	QUO	C13-C12-N11-C10
1	C	34	QUO	C16-C12-N11-C10
1	D	16	H2U	O4'-C1'-N1-C6
1	C	16	H2U	O4'-C1'-N1-C2
1	C	16	H2U	O4'-C1'-N1-C6

There are no ring outliers.

19 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	20(A)	H2U	5	0
1	D	8	4SU	5	0
1	C	20	H2U	2	0
1	C	34	QUO	6	0
1	D	54	5MU	2	0
1	D	46	G7M	5	0
1	C	65	PSU	4	0
1	D	65	PSU	2	0
1	C	46	G7M	1	0
1	D	34	QUO	7	0
1	D	16	H2U	2	0
1	C	54	5MU	3	0
1	C	37	2MA	1	0
1	D	55	PSU	1	0
1	C	16	H2U	2	0
1	D	20(A)	H2U	1	0
1	D	20	H2U	1	0
1	C	8	4SU	2	0
1	D	37	2MA	5	0

## 5.5 Carbohydrates ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	59:G	O3'	60:U	P	1.76

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	63/73 (86%)	-0.15	0 <span>100</span> <span>100</span>	26, 56, 90, 102	0
1	D	63/73 (86%)	-0.13	1 (1%) <span>72</span> <span>44</span>	32, 52, 96, 101	0
2	A	580/580 (100%)	0.01	3 (0%) <span>91</span> <span>75</span>	7, 26, 64, 102	0
2	B	580/580 (100%)	0.08	8 (1%) <span>75</span> <span>49</span>	6, 34, 68, 102	0
All	All	1286/1306 (98%)	0.03	12 (0%) <span>84</span> <span>63</span>	6, 31, 71, 102	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	437	ALA	5.7
2	A	432	ASP	5.0
2	B	580	PRO	5.0
2	B	435	GLU	4.9
1	D	72	C	2.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PSU	D	65	20/21	0.86	0.15	76,79,82,83	0
1	H2U	C	20	20/21	0.88	0.24	61,72,77,77	0
1	5MU	D	54	21/22	0.89	0.15	54,60,64,65	0
1	H2U	D	20	20/21	0.89	0.20	49,68,72,73	0
1	QUO	D	34	32/33	0.90	0.23	48,63,72,73	0
1	4SU	C	8	20/21	0.90	0.19	52,56,60,61	0
1	5MU	C	54	21/22	0.91	0.16	79,81,81,82	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	H2U	D	20(A)	20/21	0.93	0.15	57,61,66,67	0
1	PSU	D	55	20/21	0.93	0.15	48,53,65,65	0
1	H2U	C	16	20/21	0.93	0.14	60,66,70,73	0
1	PSU	C	55	20/21	0.93	0.10	74,75,82,82	0
1	QUO	C	34	32/33	0.94	0.25	23,35,51,53	0
1	G7M	D	46	24/25	0.94	0.16	43,47,49,53	0
1	PSU	C	65	20/21	0.94	0.12	72,75,80,82	0
1	H2U	D	16	20/21	0.95	0.18	51,65,67,71	0
1	4SU	D	8	20/21	0.95	0.20	39,43,47,48	0
1	G7M	C	46	24/25	0.95	0.18	36,42,48,50	0
1	H2U	C	20(A)	20/21	0.95	0.14	57,63,73,73	0
1	2MA	D	37	23/24	0.95	0.17	50,60,67,68	0
1	2MA	C	37	23/24	0.96	0.18	25,41,44,64	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.