



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:23 AM GMT

PDB ID : 3AL0  
Title : Crystal structure of the glutamine transamidosome from *Thermotoga maritima* in the glutamylation state.  
Authors : Ito, T.; Yokoyama, S.  
Deposited on : 2010-07-19  
Resolution : 3.37 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

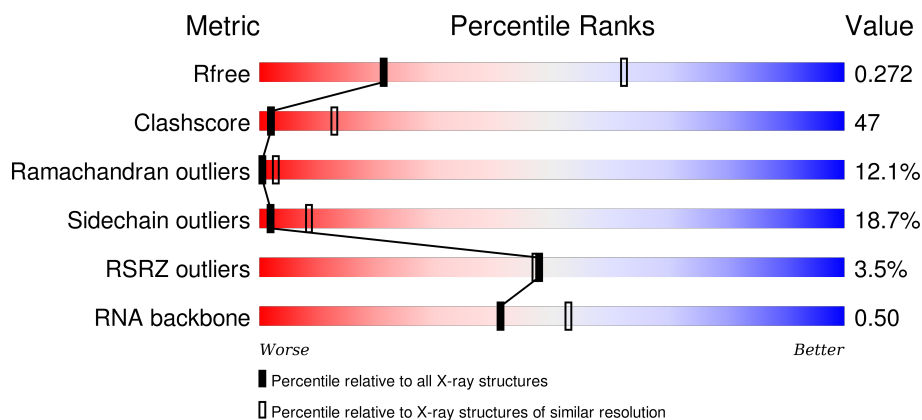
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.37 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))
$R_{free}$	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)
RNA backbone	2183	1016 (3.92-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	475	<div> <div>4%</div> <div>26% 54% 18%</div> <div>..</div> </div>
2	B	482	<div> <div>5%</div> <div>29% 47% 21%</div> <div>.</div> </div>
3	C	592	<div> <div>2%</div> <div>29% 50% 14%</div> <div>• 5%</div> </div>
4	E	74	<div> <div></div> <div>32% 54% 9%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GSU	C	1001	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13869 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 protein called Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3672	2342	625	690	15			

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	482	Total	C	N	O	S	0	0	0
			3891	2462	662	744	23			

- Molecule 3 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit C, Glutamyl-tRNA synthetase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	564	Total	C	N	O	S	0	0	0
			4692	3007	794	874	17			

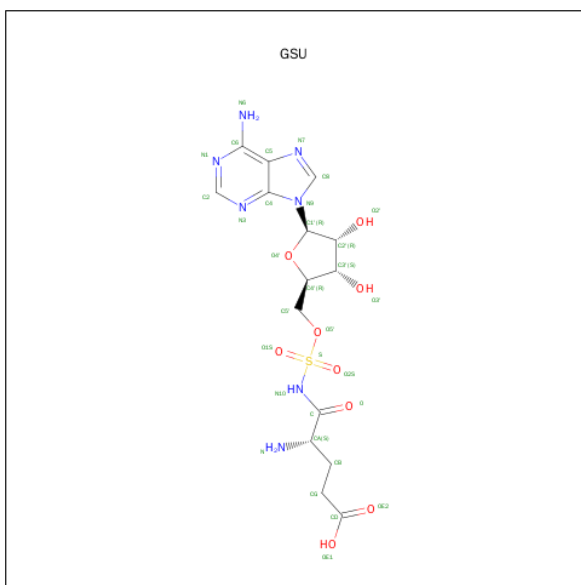
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	EXPRESSION TAG	UNP Q9WY94
C	1	GLY	-	EXPRESSION TAG	UNP Q9WY94

- Molecule 4 is a RNA chain called tRNA<sup>Gln</sup>.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	74	Total	C	N	O	P	0	0	0
			1581	703	281	523	74			

- Molecule 5 is O5'-(L-GLUTAMYL-SULFAMOYL)-ADENOSINE (three-letter code: GSU) (formula: C<sub>15</sub>H<sub>21</sub>N<sub>7</sub>O<sub>9</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	S	0	0
			32	15	7	9	1		

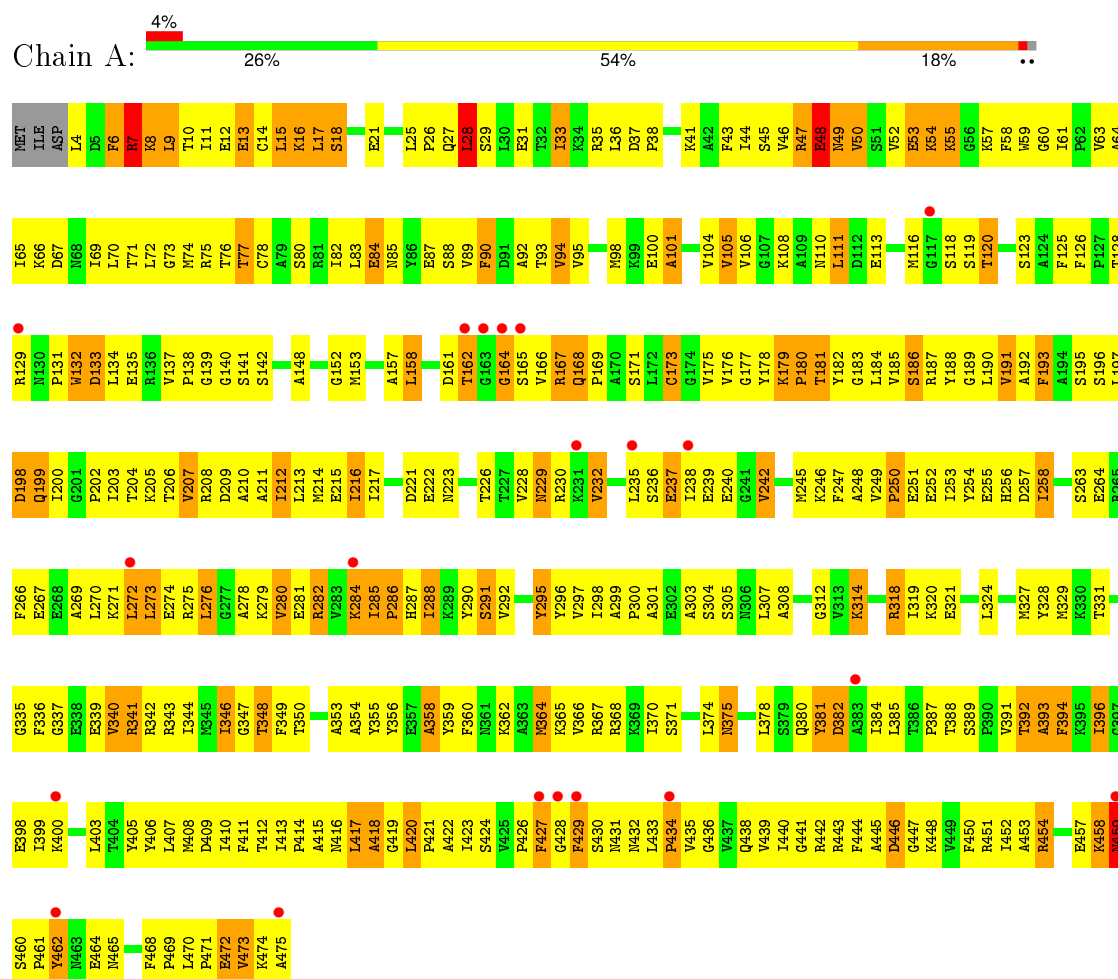
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Zn 1 1	0	0

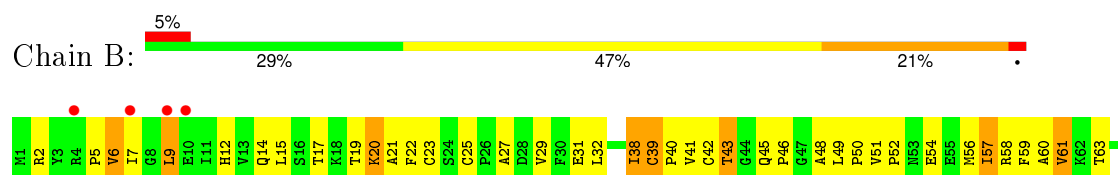
### 3 Residue-property plots

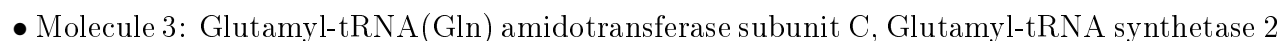
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

#### • Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A



#### • Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

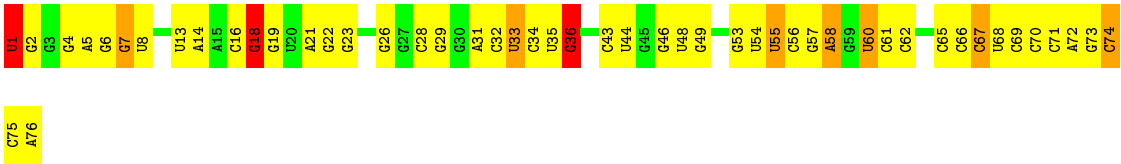




S478	K410	G339	K278	P206	R152	ME1
Q479	D411	W340	G279	Y207	F133	ME2
L480	I412	E341	Y280	R208	A134	ME3
Y481	S413	A342	M281	E211	P135	K3
D482	M414	K343	E282	R212	G66	Y4
L483	K415	W344	F283	L213	P137	T5
M484	G416	F345	D284	E214	T138	K6
Y485	K346	K346	D285	L213	G139	D7
F486	K347	K347	E286	Y216	L140	L8
F487	K348	K348	T287	R217	L141	V9
Q488	K349	K349	L288	E218	H142	L10
M489	L350	L350	E289	Y219	V143	H11
E425	L351	L351	L292	A220	G144	L12
D490	L352	L352	L293	E221	K78	E13
Y492	F491	F491	M294	R222	A146	K79
G493	M428	D365	K295	L223	R147	N14
Y494	H431	R356	E296	V224	T148	
E495	M432	T357	E297	E225	A149	R17
K496	R433	F358	G298	D226	L150	L18
D497	K434	S360	F299	R228	F151	E19
Y498	L435	K361	P300	A229	M154	L20
F499	D436	R362	T301	E229	F155	S21
F502	L437	H363	Y302	V233	T94	E22
L503	E438	T366	M303	Y234	HIS	D23
M504	L439	F304	A305	D236	ARG	Q24
R505	L440	E369	Y306	E237	GLY	R25
E506	K441	H370	V307	D238	SER	S27
E507	R442	F371	V308	P239	GLY	L28
A508	E443	R372	D309	E240	SER	K29
E509	L444	E374	D310	K241	GLY	K30
R510	D446	G375	H311	E242	SER	D31
L512	W447	L376	L312	T244	GLY	Q33
E513	A448	L377	R314	T245	SER	Q34
E514	K453		L315	E246	MET	I35
A515	E454	K382	S316	Y247	PHE	L36
L518	L455	K383	G317	E248	THR	D37
F519	E456	L388	F318	Y249	GLY	Y38
K520	S457	F319	V319	P250	ALA	V39
E521	V458	G389	R320	E251	PHE	E40
L522	D459	W390	G321	K254	ASP	L41
M523	E460	R391	E322	L183	ILE	L42
S524	R461	V392	D323	L184	LEU	M43
W525	Y462	E393	H324	E258	LEU	V44
F463	F463	L325	L325	P259	VAL	D46
M526	E464	S326	S326	V260	GLY	V47
M527	E465	F398	K327	T261	P119	E48
E528	F466	T399	T328	V266	K120	G49
E529	L467	L400	P329	L267	K121	V50
E531	L469	E401	K330	L267	L192	E51
L534	C470	K403	Q331	K270	L193	P52
R535	R471	L404	L332		D199	N53
D536	E472	Q405	T334	F273	L200	T55
L537	K473	S406	V335	E274	L128	P56
S538	F407	E336	E336	D275	V129	V57
E539	T476	D408	A337	L276	R130	E58
E540	L477	E408	E338	L276	F204	D59
					G295	S60



● Molecule 4: tRNA<sup>Gln</sup>





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.95Å 125.66Å 313.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.67 – 3.37 48.67 – 3.37	Depositor EDS
% Data completeness (in resolution range)	92.7 (48.67-3.37) 92.7 (48.67-3.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.11 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, $R_{free}$	0.195 , 0.269 0.195 , 0.272	Depositor DCC
$R_{free}$ test set	2068 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.0	Xtriage
Anisotropy	0.952	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 99.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 40830 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13869	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, GSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.31	0/3740	0.54	0/5047
2	B	0.40	0/3964	0.63	0/5336
3	C	0.43	0/4798	0.65	2/6453 (0.0%)
4	E	0.84	1/1765 (0.1%)	0.93	5/2749 (0.2%)
All	All	0.47	1/14267 (0.0%)	0.66	7/19585 (0.0%)

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
4	E	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	U	OP3-P	-7.12	1.52	1.61

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	23	G	OP2-P-O3'	6.15	118.74	105.20
3	C	223	LEU	CA-CB-CG	5.33	127.55	115.30
3	C	306	VAL	CB-CA-C	-5.23	101.47	111.40
4	E	36	G	O4'-C1'-N9	-5.21	104.03	108.20
4	E	55	U	C5'-C4'-C3'	-5.13	107.80	116.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	1	U	Sidechain
4	E	18	G	Sidechain
4	E	67	C	Sidechain
4	E	7	G	Sidechain

## 5.2 Too-close contacts [i](#)

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	3672	0	3734	377	0
2	B	3891	0	3905	444	0
3	C	4692	0	4654	429	0
4	E	1581	0	800	68	0
5	C	32	0	20	11	0
6	B	1	0	0	0	0
All	All	13869	0	13113	1258	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 47.

The worst 5 of 1258 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:546:LYS:NZ	4:E:35:U:H5'	1.59	1.16
1:A:8:LYS:HB3	1:A:470:LEU:HD12	1.38	1.05
1:A:52:VAL:HG22	1:A:104:VAL:HG11	1.32	1.05
4:E:6:G:H2'	4:E:7:G:H5'	1.36	1.04
1:A:378:LEU:HG	1:A:442:ARG:HA	1.40	1.01

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	
1	A	470/475 (99%)	305 (65%)	113 (24%)	52 (11%)	0	4
2	B	480/482 (100%)	306 (64%)	102 (21%)	72 (15%)	0	1
3	C	560/592 (95%)	396 (71%)	105 (19%)	59 (10%)	1	4
All	All	1510/1549 (98%)	1007 (67%)	320 (21%)	183 (12%)	0	3

5 of 183 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	55	LYS
1	A	101	ALA
1	A	120	THR
1	A	133	ASP

### 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	
1	A	394/397 (99%)	324 (82%)	70 (18%)	2	10
2	B	430/430 (100%)	349 (81%)	81 (19%)	2	8
3	C	510/530 (96%)	412 (81%)	98 (19%)	2	7
All	All	1334/1357 (98%)	1085 (81%)	249 (19%)	2	8

5 of 249 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	226	PHE
2	B	374	GLN
3	C	471	ARG
2	B	255	TRP
2	B	320	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	374	GLN
3	C	33	GLN
3	C	489	ASN
2	B	435	GLN
1	A	375	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	E	73/74 (98%)	11 (15%)	1 (1%)

5 of 11 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	E	8	U
4	E	16	C
4	E	18	G
4	E	22	G
4	E	26	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	E	73	G

## 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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	GSU	C	1001	-	24,34,34	0.91	1 (4%)	30,50,50	2.17	6 (20%)

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
5	GSU	C	1001	-	-	0/16/40/40	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1001	GSU	O4'-C1'	2.38	1.44	1.41

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1001	GSU	N3-C2-N1	-8.86	122.11	128.89
5	C	1001	GSU	C5'-O5'-S	-3.73	110.88	118.02
5	C	1001	GSU	O2S-S-N10	-3.21	104.21	108.50
5	C	1001	GSU	C4-C5-N7	-2.87	106.84	109.48
5	C	1001	GSU	CA-C-N10	2.10	119.09	114.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1001	GSU	11	0

## 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 ⓘ

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	A	472/475 (99%)	0.23	20 (4%) 40 39	83, 143, 190, 241	0
2	B	482/482 (100%)	0.20	25 (5%) 31 30	51, 114, 185, 262	0
3	C	564/592 (95%)	-0.05	11 (1%) 68 68	52, 106, 178, 224	0
4	E	74/74 (100%)	-0.43	0 100 100	70, 91, 146, 167	0
All	All	1592/1623 (98%)	0.09	56 (3%) 48 47	51, 121, 185, 262	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	210	GLY	11.5
2	B	209	THR	11.0
2	B	212	GLN	8.7
1	A	427	PHE	6.8
3	C	529	GLU	5.4

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ZN	B	1001	1/1	0.98	0.20	0.17	81,81,81,81	0
5	GSU	C	1001	32/32	0.95	0.21	-0.04	48,78,102,109	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.