wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 02:07 AM EDT

PDB ID	:	1N77
Title	:	Crystal structure of Thermus thermophilus glutamyl-tRNA synthetase complexed with tRNA(Glu) and ATP.
Authors	:	Sekine, S.; Nureki, O.; Dubois, D.Y.; Bernier, S.; Chenevert, R.; Lapointe, J.; Vassylyev, D.G.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2002-11-13
Resolution	:	2.40 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

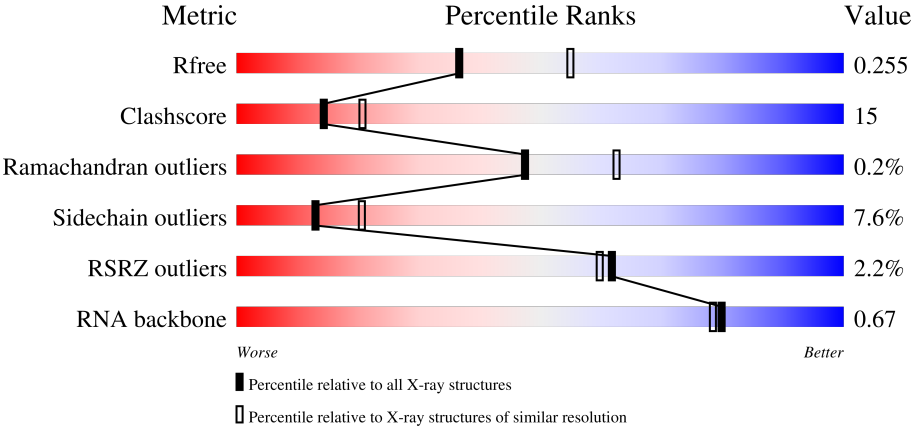
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	75	.% 52% 29% 13% 5%
1	D	75	5% 44% 35% 16% 5%
2	A	468	.% 69% 28% .
2	B	468	3% 63% 33% .

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11391 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 tRNA(Glu).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	75	1597	711	284	527	75	0	0	0
1	D	75	1597	711	284	527	75	0	0	0

- Molecule 2 is a protein called Glutamyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	468	3814	2443	676	687	8	0	0	0
2	B	468	3814	2443	676	687	8	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

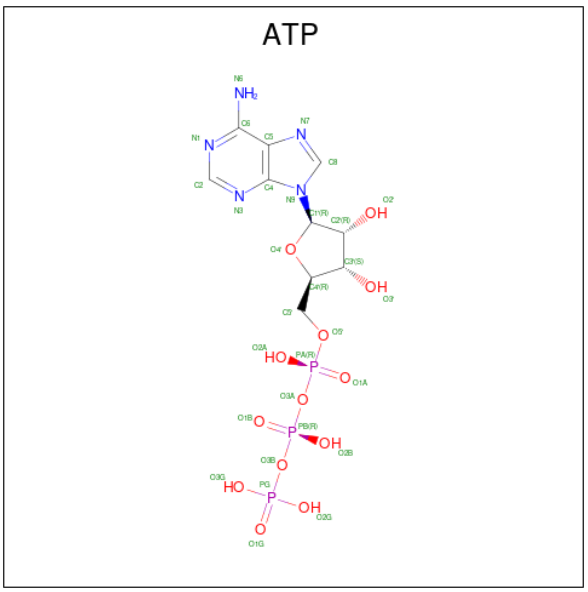
Chain	Residue	Modelled	Actual	Comment	Reference
A	74	GLY	ALA	SEE REMARK 999	UNP P27000
A	75	GLY	ALA	SEE REMARK 999	UNP P27000
A	77	HIS	THR	SEE REMARK 999	UNP P27000
B	74	GLY	ALA	SEE REMARK 999	UNP P27000
B	75	GLY	ALA	SEE REMARK 999	UNP P27000
B	77	HIS	THR	SEE REMARK 999	UNP P27000

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	C	1	1	1	0	0
3	D	1	1	1	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

$C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	70	Total	O	0	0
			70	70		
5	D	75	Total	O	0	0
			75	75		
5	A	175	Total	O	0	0
			175	175		
5	B	185	Total	O	0	0
			185	185		

3 Residue-property plots (i)

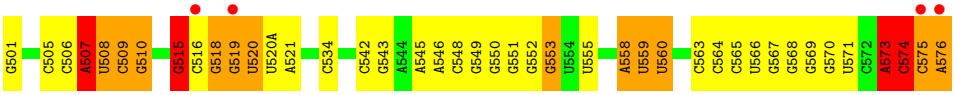
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: tRNA(Glu)

Chain C:

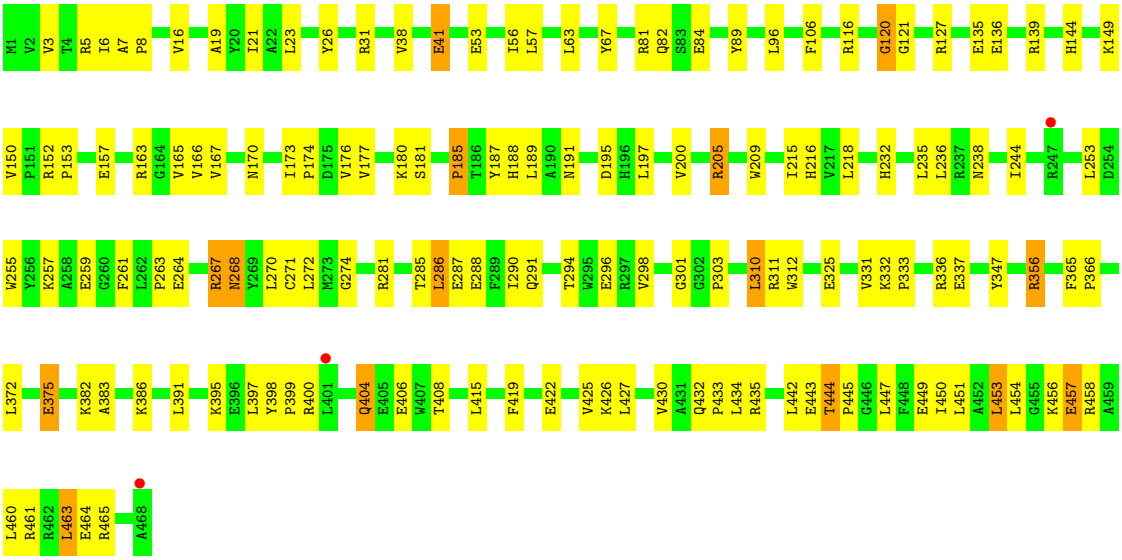
- Molecule 1: tRNA(Glu)

Chain D:



- Molecule 2: Glutamyl-tRNA synthetase

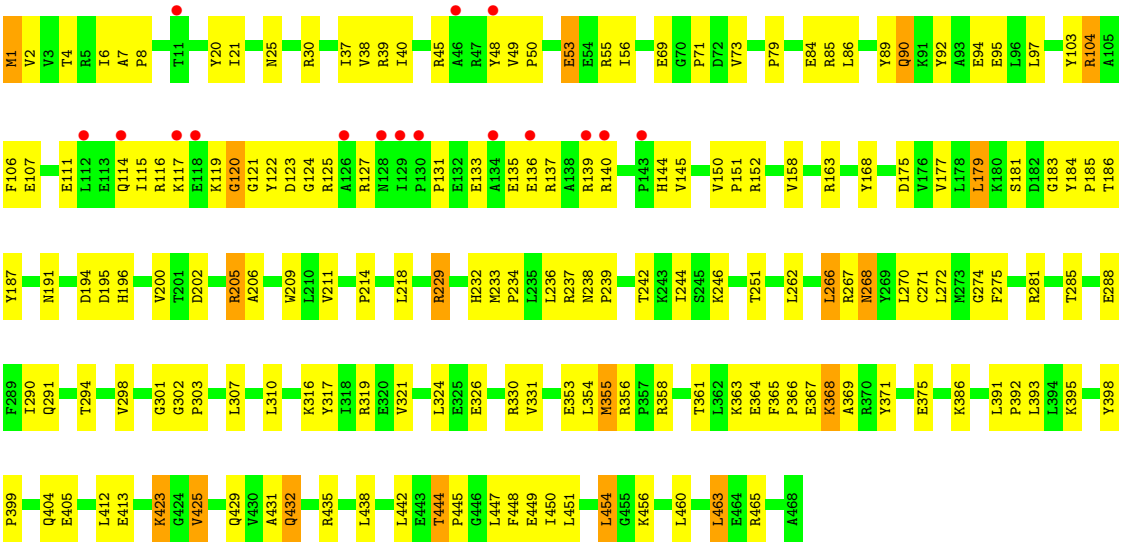
Chain A:



- Molecule 2: Glutamyl-tRNA synthetase

Chain B:

3%
63%
33%


M1 V2 V3 T4 R5 I6 A7 P8 T11 Y20 I21 N25 R30 I37 V38 R39 I40 R45 A46 R47 Y48 V49 P50 E53 E54 R55 I56 E69 G70 P71 D72 V73 P79 E84 R85 L86 Y89 Q90 K91 Y92 A93 E94 E95 L96 L97 Y103 R104 A105
F106 E107 E111 L112 E113 Q114 I115 R116 K117 E118 K119 G120 G121 Y122 D123 G124 R125 A126 R127 N128 I129 P130 P131 E132 E133 A134 E135 E136 R137 A138 R139 R140 P143 H144 V145 V150 P151 R152 V158 R163 Y168 D175 V176 V177 L178 L179 K180 S181 D182 G183 Y184 P185 T186
Y187 N191 D194 D195 H196 V200 T201 D202 R205 A206 W209 L210 V211 P214 L218 R229 H232 M233 P234 L235 L236 R237 N238 P239 T242 K243 I244 S245 K246 T251 L262 L266 R267 N268 Y269 L270 C271 L272 M273 G274 F275 R281 T285 E288
F289 I290 Q291 T294 V298 G301 G302 P303 L307 L310 K316 Y317 I318 R319 E320 V321 L324 E325 E326 R330 V331 E353 L354 M355 R356 P357 R358 T361 L362 K363 E364 F365 P366 E367 K368 A369 R370 Y371 E375 K386 L391 P392 L393 L394 K395 Y398
P399 Q404 E405 L412 E413 K423 G424 V425 Q429 V430 A431 Q432 R435 L438 L442 E443 T444 P445 G446 L447 F448 E449 I450 L451 L454 G455 K456 L460 L463 E464 R465 A468

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	110.69Å 219.12Å 135.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 2.40 49.40 – 2.38	Depositor EDS
% Data completeness (in resolution range)	91.4 (49.40-2.40) 90.1 (49.40-2.38)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.37Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.257 0.210 , 0.255	Depositor DCC
R_{free} test set	2972 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11391	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG

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	0.40	1/1782 (0.1%)	0.83	7/2774 (0.3%)
1	D	0.41	1/1782 (0.1%)	0.84	10/2774 (0.4%)
2	A	0.39	0/3910	0.62	0/5293
2	B	0.38	0/3910	0.60	0/5293
All	All	0.39	2/11384 (0.0%)	0.70	17/16134 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	1	1
All	All	1	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	501	G	OP3-P	-7.07	1.52	1.61
1	D	501	G	OP3-P	-6.92	1.52	1.61

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	574	C	C2'-C3'-O3'	8.50	128.20	109.50
1	D	574	C	C2'-C3'-O3'	7.52	126.04	109.50
1	C	518	G	C2'-C3'-O3'	7.40	125.78	109.50
1	C	519	G	C2'-C3'-O3'	7.32	125.60	109.50
1	D	515	G	C2'-C3'-O3'	7.30	125.57	109.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	515	G	C3'

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	515	G	Sidechain
1	D	515	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	C	1597	0	813	28	0
1	D	1597	0	813	43	0
2	A	3814	0	3818	125	0
2	B	3814	0	3818	137	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	12	4	0
4	B	31	0	12	4	0
5	A	175	0	0	6	0
5	B	185	0	0	8	0
5	C	70	0	0	0	0
5	D	75	0	0	6	0
All	All	11391	0	9286	312	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 15.

The worst 5 of 312 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:506:C:O2'	1:D:507:A:H5'	1.72	0.89
2:B:454:LEU:HD22	2:B:454:LEU:H	1.38	0.89
1:D:576:A:H3'	2:B:209:TRP:HH2	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:205:ARG:HD3	2:A:232:HIS:CE1	2.10	0.85
2:B:454:LEU:HD22	2:B:454:LEU:N	1.91	0.85

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	466/468 (100%)	450 (97%)	15 (3%)	1 (0%)	47	62
2	B	466/468 (100%)	449 (96%)	16 (3%)	1 (0%)	47	62
All	All	932/936 (100%)	899 (96%)	31 (3%)	2 (0%)	47	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	120	GLY
2	B	120	GLY

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	393/393 (100%)	366 (93%)	27 (7%)	15	25
2	B	393/393 (100%)	360 (92%)	33 (8%)	11	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	786/786 (100%)	726 (92%)	60 (8%)	13 20

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	53	GLU
2	B	432	GLN
2	B	191	ASN
2	B	425	VAL
2	B	463	LEU

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

Mol	Chain	Res	Type
2	B	25	ASN
2	B	171	GLN
2	B	432	GLN
2	B	232	HIS
2	B	404	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	16 (21%)	9 (12%)
1	D	74/75 (98%)	14 (18%)	9 (12%)
All	All	148/150 (98%)	30 (20%)	18 (12%)

5 of 30 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	507	A
1	C	508	U
1	C	510	G
1	C	515	G
1	C	516	C

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	558	A

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Mol	Chain	Res	Type
1	D	574	C
1	D	573	A
1	C	574	C
1	D	519	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	B	601	-	26,33,33	0.66	0	31,52,52	1.44	7 (22%)
4	ATP	A	600	-	26,33,33	0.66	0	31,52,52	1.48	7 (22%)

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
4	ATP	B	601	-	-	6/18/38/38	0/3/3/3
4	ATP	A	600	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	ATP	PB-O3B-PG	-3.52	120.75	132.83
4	A	600	ATP	PA-O3A-PB	-3.36	121.31	132.83
4	B	601	ATP	PA-O3A-PB	-3.28	121.57	132.83
4	A	600	ATP	PB-O3B-PG	-3.21	121.80	132.83
4	A	600	ATP	O3'-C3'-C2'	2.82	120.93	111.82

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	ATP	C5'-O5'-PA-O1A
4	A	600	ATP	C5'-O5'-PA-O2A
4	B	601	ATP	C5'-O5'-PA-O2A
4	B	601	ATP	C5'-O5'-PA-O3A
4	B	601	ATP	C5'-O5'-PA-O1A

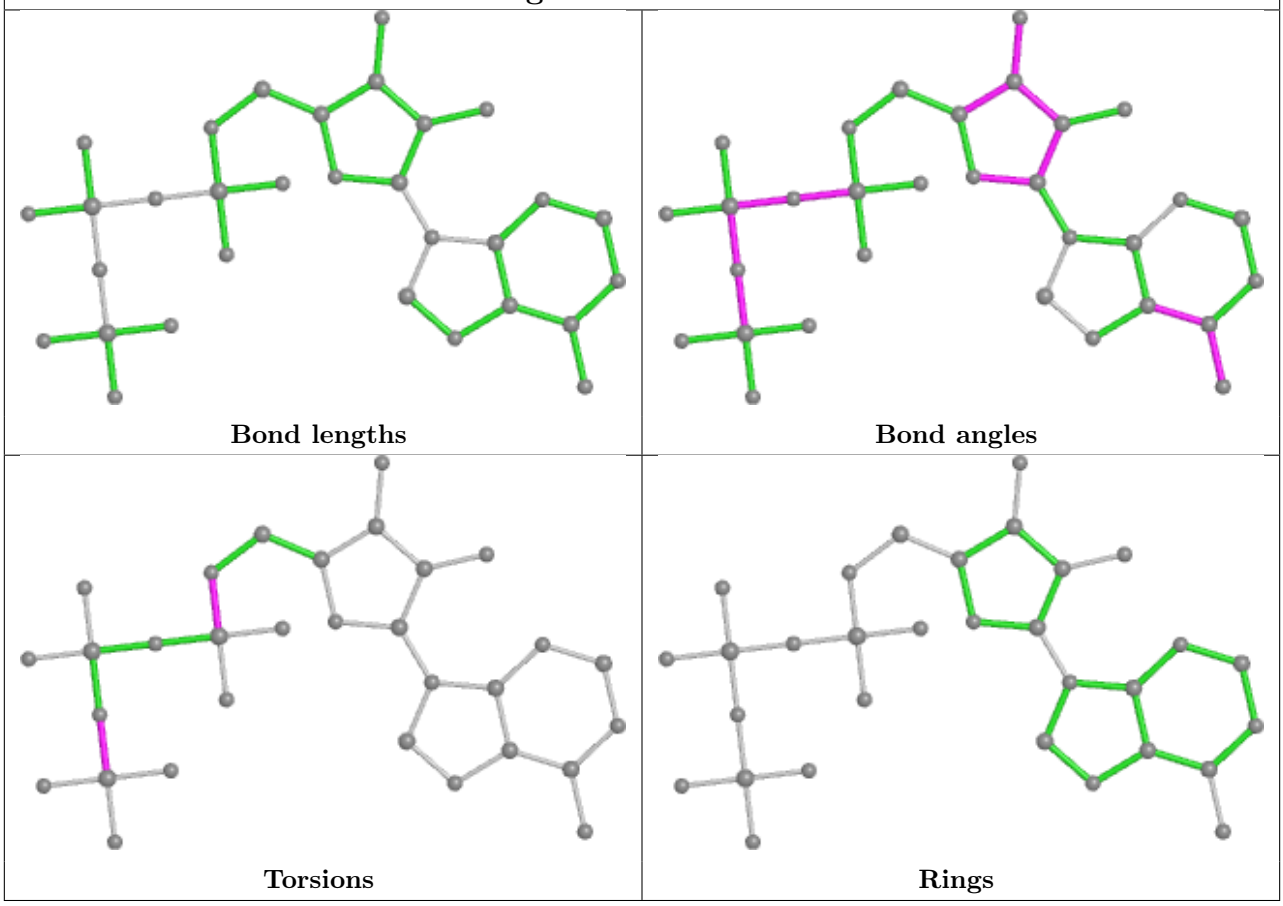
There are no ring outliers.

2 monomers are involved in 8 short contacts:

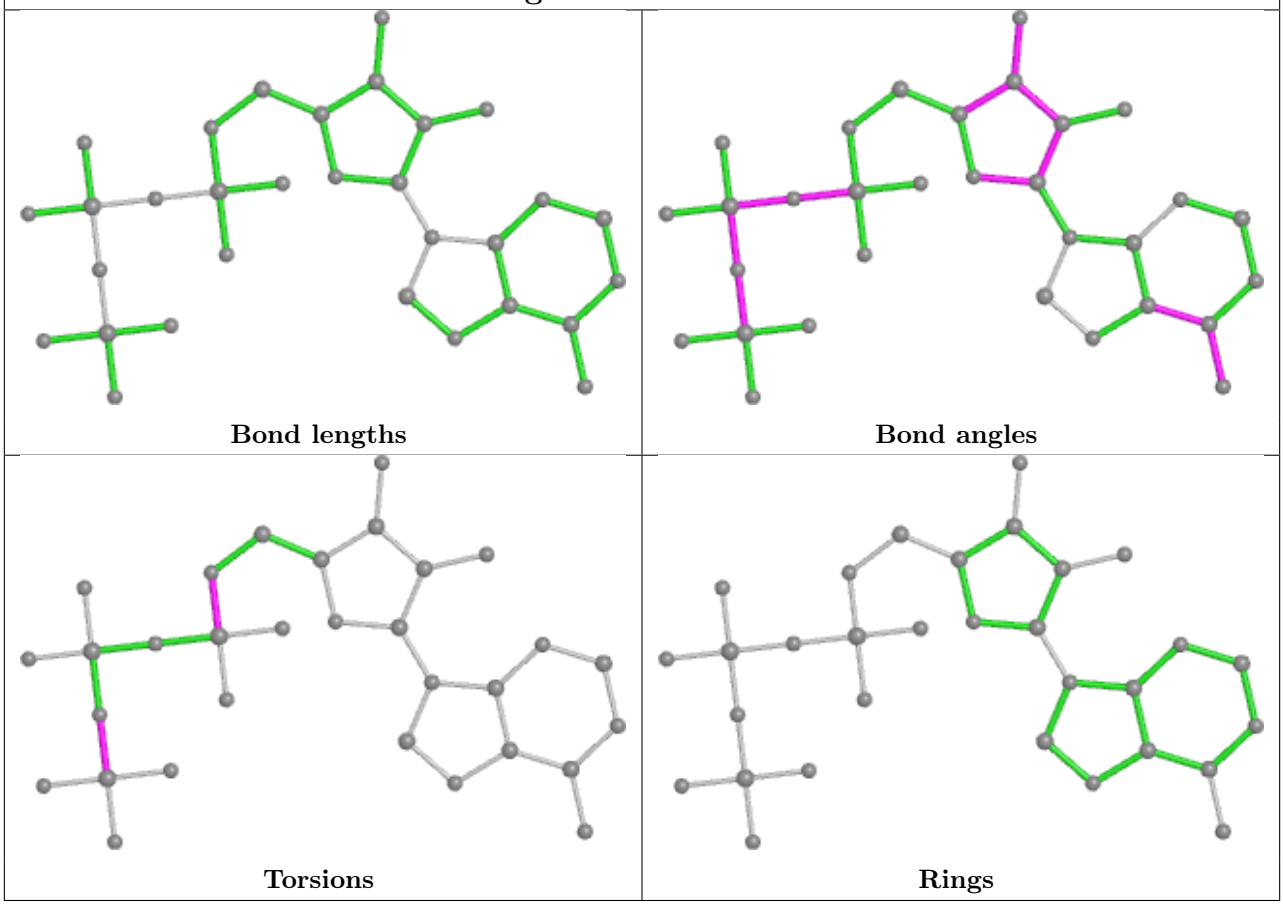
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	ATP	4	0
4	A	600	ATP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP B 601



Ligand ATP A 600



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 (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, 95th 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^2)	Q<0.9
1	C	75/75 (100%)	-0.50	1 (1%)	77	75	27, 48, 85, 104	0
1	D	75/75 (100%)	-0.25	4 (5%)	26	25	25, 49, 96, 113	0
2	A	468/468 (100%)	-0.42	3 (0%)	89	88	12, 27, 58, 73	0
2	B	468/468 (100%)	-0.31	16 (3%)	45	44	12, 30, 79, 93	0
All	All	1086/1086 (100%)	-0.37	24 (2%)	62	60	12, 31, 80, 113	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	576	A	4.7
2	B	129	ILE	4.0
2	B	48	TYR	3.8
2	B	11	THR	3.5
2	B	140	ARG	3.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

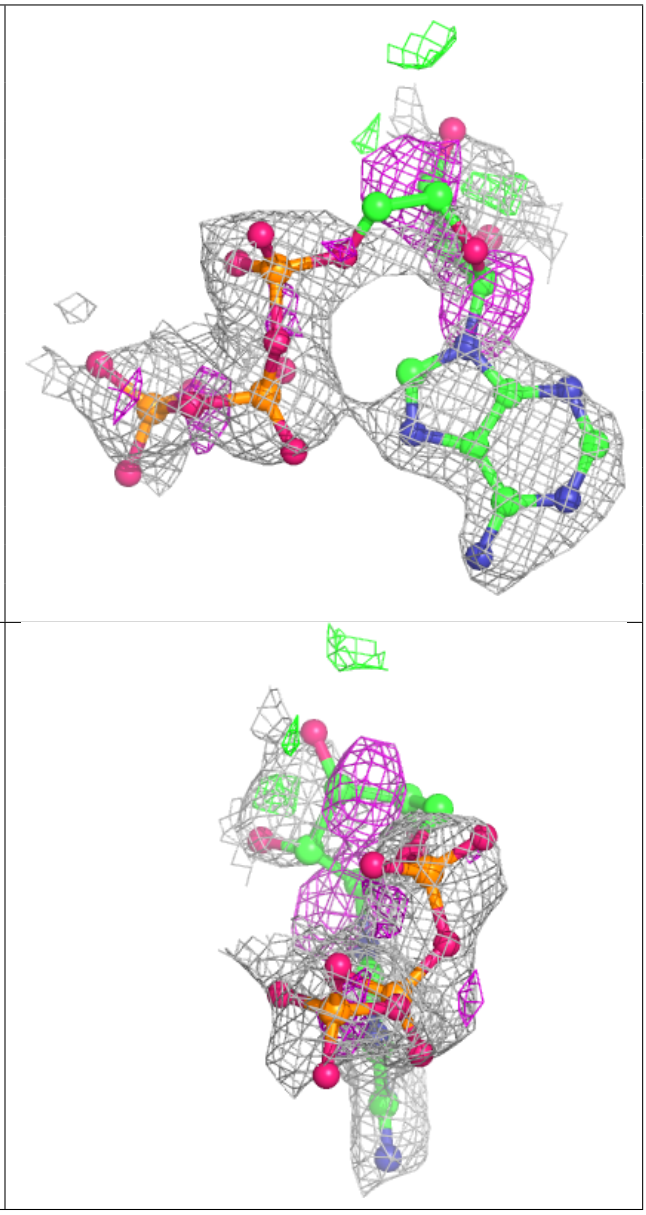
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ATP	A	600	31/31	0.71	0.30	76,86,104,105	0
4	ATP	B	601	31/31	0.80	0.29	84,94,110,111	0
3	MG	C	700	1/1	0.95	0.27	38,38,38,38	0
3	MG	D	701	1/1	0.97	0.27	39,39,39,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

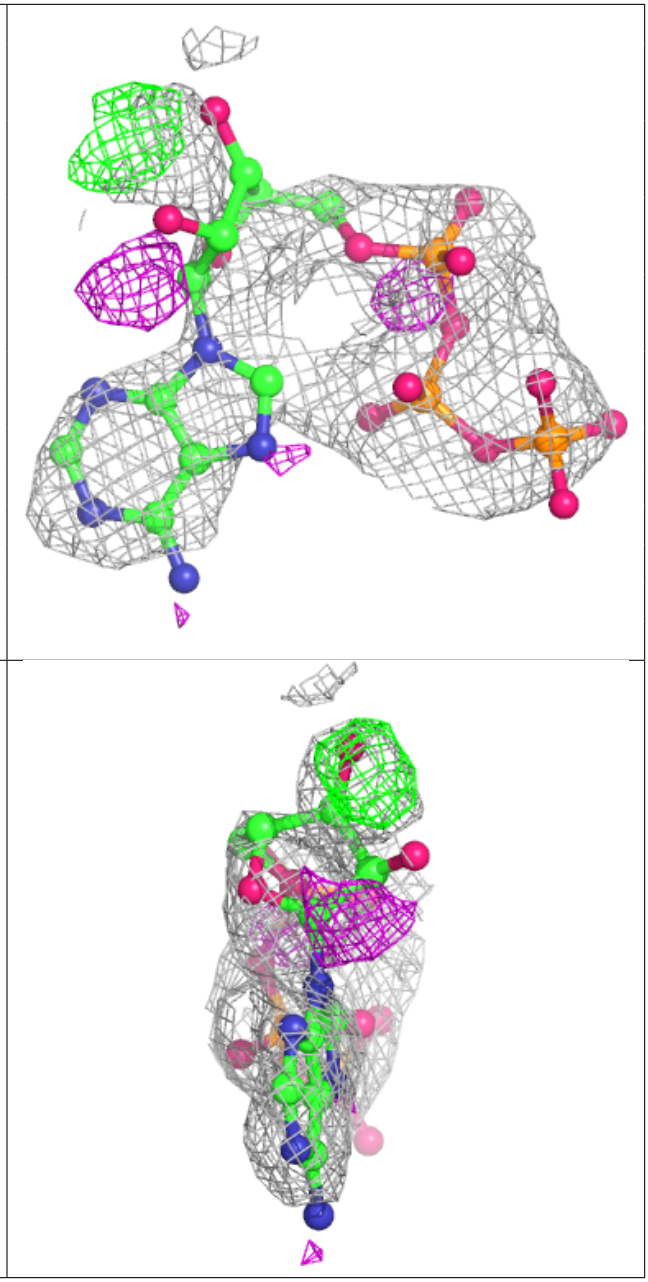
Electron density around ATP A 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ATP B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.