

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 15, 2023 – 01:06 PM EDT

PDB ID	:	8DQJ
Title	:	Crystal structure of pyrrolysyl-tRNA synthetase from Methanomethylophilus
		alvus engineered for acridone amino acid (AST) bound to ATP and acridone
Authors	:	Gottfried-Lee, I.; Karplus, P.A.; Mehl, R.A.; Cooley, R.B.
Deposited on	:	2022-07-19
Resolution	:	1.54  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 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 (1)) were used in the production of this report:

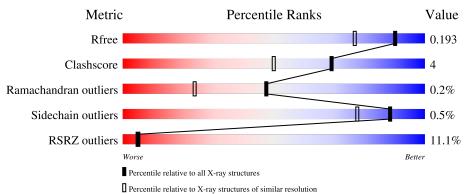
MolProbity Mogul Xtriage (Phenix) EDS	:	4.02b-467 1.8.5 (274361), CSD as541be (2020) 1.13 2.36
buster-report Percentile statistics Refmac	: : :	1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 1.54 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	2556 (1.56-1.52)
Clashscore	141614	2634(1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	А	276	84% 7%	9%	i
1	D	276	90%	8% •	i



#### 8DQJ

# 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8541 atoms, of which 4027 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.

Mol	Chain	Residues			Atom	s	ZeroOcc	AltConf	Trace		
1	1 D 271	Total	С	Η	Ν	0	S	0	0	0	
		271	4173	1328	2064	353	413	15	0	0	0
1	Δ	051	Total	С	Η	Ν	0	S	0	11	0
	A	251	3855	1232	1915	318	376	14	0		

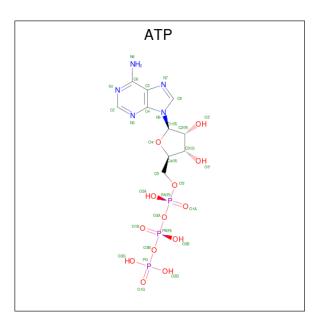
• Molecule 1 is a protein called AA\_TRNA\_LIGASE\_II domain-containing protein.

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP A0A3G3IHP7
D	1	GLY	-	expression tag	UNP A0A3G3IHP7
D	166	SER	ASN	engineered mutation	UNP A0A3G3IHP7
D	168	CYS	VAL	engineered mutation	UNP A0A3G3IHP7
D	239	THR	TRP	engineered mutation	UNP A0A3G3IHP7
А	0	SER	-	expression tag	UNP A0A3G3IHP7
А	1	GLY	-	expression tag	UNP A0A3G3IHP7
А	166	SER	ASN	engineered mutation	UNP A0A3G3IHP7
А	168	CYS	VAL	engineered mutation	UNP A0A3G3IHP7
А	239	THR	TRP	engineered mutation	UNP A0A3G3IHP7

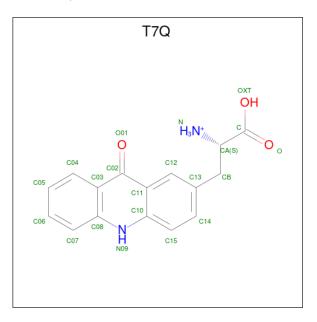
• Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).





Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total 42	C 10	H 11	N 5	O 13	Р 3	0	0

• Molecule 3 is (2 {S})-2-azanyl-3-(9-oxidanylidene-10 {H}-acridin-2-yl)propanoic acid (three-letter code: T7Q) (formula: C<sub>16</sub>H<sub>15</sub>N<sub>2</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



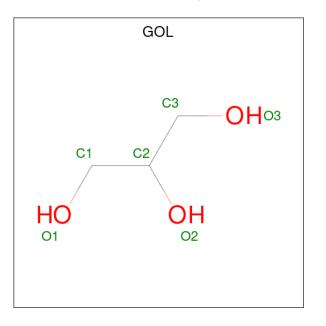
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	Л	1	Total	С	Η	Ν	Ο	0	0
5	D	1	34	16	13	2	3	0	U

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



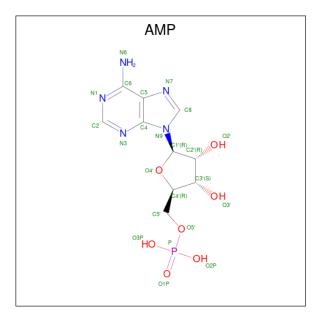
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	3	Total Mg 3 3	0	0

• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total         C         H         O           9         3         3         3	0	0

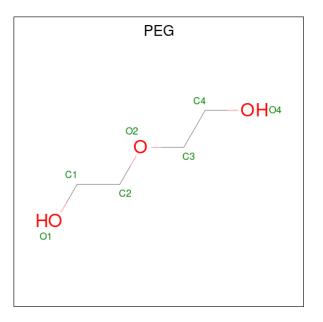
• Molecule 6 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	А	1	Total 34	C 10	H 11	N 5	O 7	Р 1	0	0

• Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf
7	А	1	Total	С	H	0	0	0
			17	4	10	3		

• Molecule 8 is water.

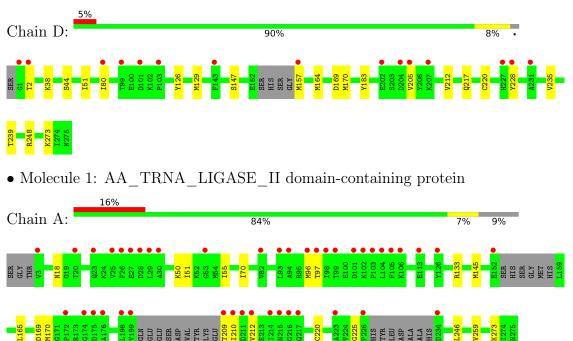
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	204	Total         O           204         204	0	0
8	А	170	Total O 170 170	0	0



## 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: AA\_TRNA\_LIGASE\_II domain-containing protein





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants	110.72Å 110.72Å 114.16Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.12 - 1.54	Depositor
Resolution (A)	35.12 - 1.54	EDS
% Data completeness	99.9 (35.12-1.54)	Depositor
(in resolution range)	99.9 (35.12 - 1.54)	EDS
R <sub>merge</sub>	0.10	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$\frac{R_{sym}}{\langle I/\sigma(I) \rangle^{-1}}$	$1.28 (at 1.54 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D	0.170 , $0.193$	Depositor
$R, R_{free}$	0.170 , $0.193$	DCC
$R_{free}$ test set	5094 reflections $(5.03\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	26.0	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.40 , $49.4$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.48, < L^2 > = 0.31$	Xtriage
	0.004 for l,-k,h	
	0.012 for -l,-k,-h	
Estimated twinning fraction	0.013 for -h,-l,-k	Xtriage
	0.005 for -h,l,k	
	0.028 for -h,k,-l	
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8541	wwPDB-VP
Average B, all atoms $(Å^2)$	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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, PEG, GOL, AMP, T7Q

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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.45	0/2001	0.66	0/2700	
1	D	0.49	0/2171	0.68	0/2931	
All	All	0.47	0/4172	0.67	0/5631	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	А	1940	1915	1908	12	0
1	D	2109	2064	2051	19	0
2	D	31	11	12	1	0
3	D	21	13	0	0	0
4	D	3	0	0	0	0
5	А	6	3	7	1	0
6	А	23	11	12	0	0
7	А	7	10	10	0	0
8	А	170	0	0	2	0
8	D	204	0	0	2	0
All	All	4514	4027	4000	30	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 4.

All (30) 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:A:51[B]:ILE:HD11	1:A:273:LYS:O	1.78	0.83
1:D:170:MET:HE3	1:D:235:VAL:HG22	1.74	0.70
1:D:80:ILE:HD11	1:A:55:ILE:HA	1.83	0.60
1:D:235:VAL:HG11	1:D:239:THR:HG21	1.84	0.59
1:A:96:MET:O	1:A:97:THR:OG1	2.18	0.55
1:D:51:ILE:HD11	1:D:273:LYS:O	2.07	0.55
1:A:70:ILE:HG21	1:A:165:LEU:HD22	1.90	0.54
1:D:164[B]:MET:SD	2:D:301:ATP:H5'1	2.50	0.52
1:A:50[A]:LYS:NZ	8:A:404:HOH:O	2.44	0.50
1:A:133:ARG:HG3	1:A:170:MET:SD	2.52	0.49
1:D:157:MET:HE3	1:D:248:ARG:CG	2.44	0.48
1:D:169:ASP:OD2	1:D:183:TYR:OH	2.25	0.48
1:A:145[B]:MET:HG2	1:A:246:LEU:HD11	1.95	0.47
1:A:259:VAL:O	1:A:259:VAL:HG22	2.14	0.47
1:D:157:MET:HE3	1:D:248:ARG:HG2	1.96	0.46
1:D:170:MET:HE2	1:D:235:VAL:HG13	1.99	0.45
1:D:170:MET:HG3	1:D:239:THR:HG22	1.99	0.45
1:D:170:MET:CE	1:D:235:VAL:HG13	2.47	0.45
1:D:157:MET:HE1	1:D:217:GLN:HG2	2.00	0.43
1:A:169[B]:ASP:OD1	1:A:170:MET:N	2.51	0.43
1:A:212:VAL:HB	1:A:220:CYS:HB3	1.99	0.43
1:D:38:LYS:HG2	8:D:418:HOH:O	2.18	0.42
1:D:205:VAL:O	1:D:228:TYR:OH	2.24	0.42
1:A:209:THR:O	1:A:210:ILE:HG13	2.19	0.42
1:D:212:VAL:HB	1:D:220:CYS:HB3	2.02	0.42
1:A:18:ASN:ND2	8:A:404:HOH:O	2.52	0.42
1:D:129:MET:HE2	1:D:129:MET:HB2	1.93	0.42
1:D:2:THR:HG22	8:D:531:HOH:O	2.20	0.41
1:D:147:SER:OG	5:A:301:GOL:H2	2.21	0.41
1:D:235:VAL:HG11	1:D:239:THR:CG2	2.50	0.41

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	Perce	$\mathbf{ntiles}$
1	А	254/276~(92%)	247~(97%)	6(2%)	1 (0%)	34	13
1	D	275/276~(100%)	271~(98%)	4(2%)	0	100	100
All	All	529/552~(96%)	518 (98%)	10 (2%)	1 (0%)	47	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	225	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
1	А	204/233~(88%)	204 (100%)	0	100 100
1	D	226/233~(97%)	223~(99%)	3(1%)	69 42
All	All	430/466~(92%)	427~(99%)	3~(1%)	88 68

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	44[A]	SER
1	D	44[B]	SER
1	D	126	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are



no such sidechains identified.

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

#### 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 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	Turne	Chain	Res	Link	Bo	ond leng	$\mathbf{ths}$	В	ond ang	les
INIOI	Type	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
5	GOL	А	301	-	$5,\!5,\!5$	1.50	1 (20%)	$5,\!5,\!5$	1.03	0
6	AMP	А	302	-	22,25,25	0.87	1 (4%)	25,38,38	1.37	2 (8%)
3	T7Q	D	302	-	22,23,23	1.94	3 (13%)	32,33,33	1.79	8 (25%)
7	PEG	А	303	-	6,6,6	0.14	0	$5,\!5,\!5$	0.13	0
2	ATP	D	301	4	26,33,33	0.65	0	$31,\!52,\!52$	1.01	2 (6%)

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	GOL	А	301	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AMP	А	302	-	-	0/6/26/26	0/3/3/3
3	T7Q	D	302	-	-	4/8/8/8	0/3/3/3
7	PEG	А	303	-	-	2/4/4/4	-
2	ATP	D	301	4	-	4/18/38/38	0/3/3/3

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All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	D	302	T7Q	C08-N09	5.73	1.50	1.38
3	D	302	T7Q	C10-N09	5.51	1.50	1.38
3	D	302	T7Q	O-C	2.70	1.30	1.22
5	А	301	GOL	O2-C2	-2.60	1.35	1.43
6	А	302	AMP	C5-C4	2.44	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	D	302	T7Q	CB-C13-C14	-5.27	110.45	120.91
3	D	302	T7Q	CB-CA-N	-5.10	91.69	111.46
6	А	302	AMP	N3-C2-N1	-4.06	122.33	128.68
3	D	302	T7Q	O01-C02-C11	-3.10	116.37	120.91
6	А	302	AMP	C2-N1-C6	2.66	123.30	118.75
3	D	302	T7Q	C11-C12-C13	-2.53	117.40	121.41
2	D	301	ATP	C5-C6-N6	2.42	124.02	120.35
3	D	302	T7Q	OXT-C-CA	2.23	120.99	113.38
3	D	302	T7Q	CB-C13-C12	2.18	124.18	120.44
3	D	302	T7Q	O-C-CA	-2.06	114.85	122.14
3	D	302	T7Q	CB-CA-C	2.05	122.92	111.83
2	D	301	ATP	O4'-C4'-C3'	-2.01	101.13	105.11

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	ATP	C5'-O5'-PA-O1A
2	D	301	ATP	C5'-O5'-PA-O2A
3	D	302	T7Q	C-CA-CB-C13
3	D	302	T7Q	O-C-CA-N
3	D	302	T7Q	OXT-C-CA-N
7	А	303	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
5	А	301	GOL	O1-C1-C2-C3
7	А	303	PEG	O1-C1-C2-O2
3	D	302	T7Q	N-CA-CB-C13
2	D	301	ATP	C5'-O5'-PA-O3A
5	А	301	GOL	O2-C2-C3-O3
2	D	301	ATP	C4'-C5'-O5'-PA
5	А	301	GOL	O1-C1-C2-O2

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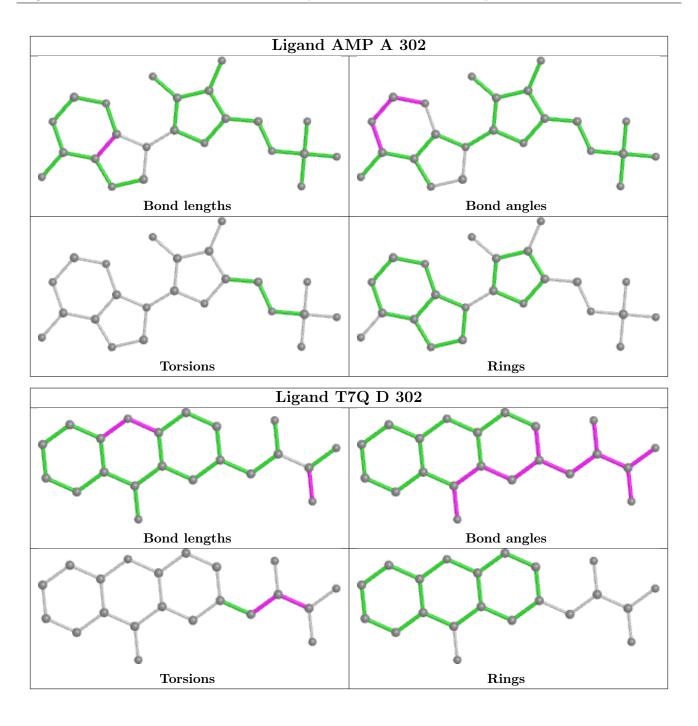
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	301	GOL	1	0
2	D	301	ATP	1	0

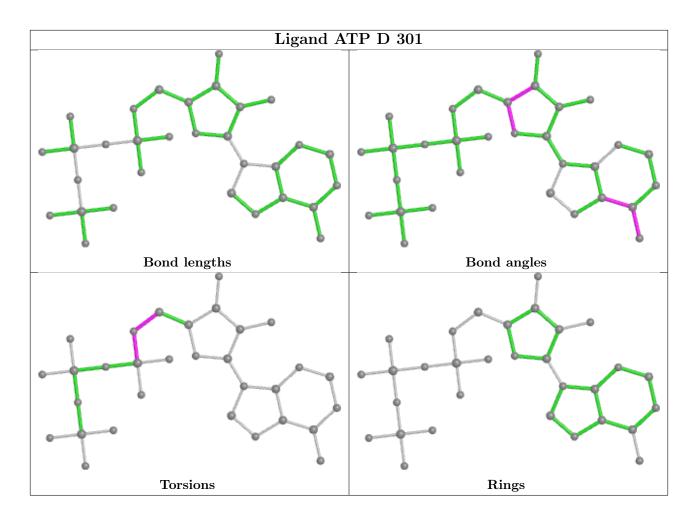
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











## 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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{A}^2)$	Q < 0.9
1	А	251/276~(90%)	0.75	43 (17%) 1 1	23, 37, 69, 85	0
1	D	271/276~(98%)	0.27	15 (5%) 25 28	20, 29, 55, 69	0
All	All	522/552~(94%)	0.50	58 (11%) 5 5	20, 33, 63, 85	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	210	ILE	5.5
1	А	101	ASP	5.4
1	А	104	LEU	5.0
1	D	228	TYR	4.6
1	А	26	PHE	4.6
1	А	126	TYR	4.3
1	D	204	ASP	4.2
1	А	103	PRO	4.1
1	А	209	THR	3.9
1	А	175	ASP	3.9
1	А	199	VAL	3.8
1	А	29	LEU	3.8
1	А	98	ILE	3.7
1	А	174	GLY	3.7
1	D	2	THR	3.7
1	А	93	LEU	3.6
1	D	99	THR	3.6
1	А	25	VAL	3.5
1	А	97	THR	3.5
1	А	226	PRO	3.4
1	А	3	VAL	3.3
1	А	28	ASP	3.3
1	А	172	PRO	3.3
1	A	23	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	205	VAL	3.2
1	А	102	LYS	3.1
1	А	176	ALA	3.0
1	D	1	GLY	2.9
1	А	94	ALA	2.9
1	А	82	VAL	2.8
1	А	99	THR	2.7
1	А	53	GLY	2.6
1	А	234	ASP	2.6
1	А	215	ASN	2.5
1	D	101	ASP	2.5
1	А	30	ALA	2.4
1	А	105	PHE	2.4
1	А	216	GLY	2.4
1	D	231	ALA	2.4
1	А	106	LYS	2.4
1	А	217	GLN	2.3
1	D	80	ILE	2.3
1	А	223	ALA	2.3
1	А	113	GLU	2.3
1	А	198	LEU	2.2
1	А	211	ASP	2.2
1	D	207	LYS	2.2
1	D	227	HIS	2.2
1	D	202	GLU	2.2
1	А	27	GLU	2.1
1	D	103	PRO	2.1
1	А	152	GLU	2.1
1	D	157	MET	2.1
1	D	143	PHE	2.1
1	А	96	MET	2.0
1	А	212	VAL	2.0
1	А	214	ILE	2.0
1	А	20	THR	2.0

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### 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.

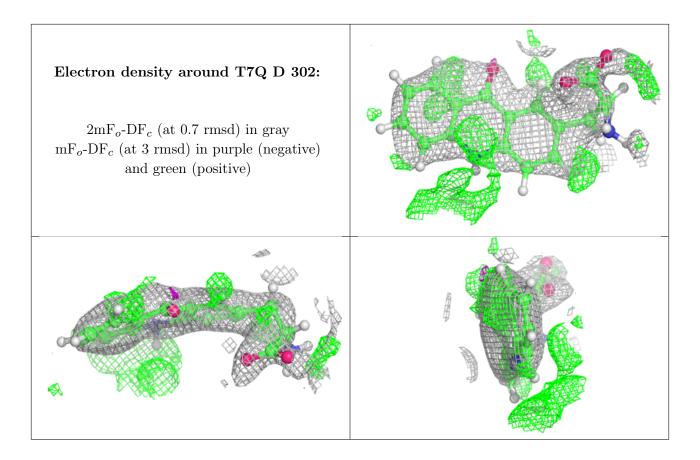
### 6.4 Ligands (i)

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,  $95^{th}$  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.

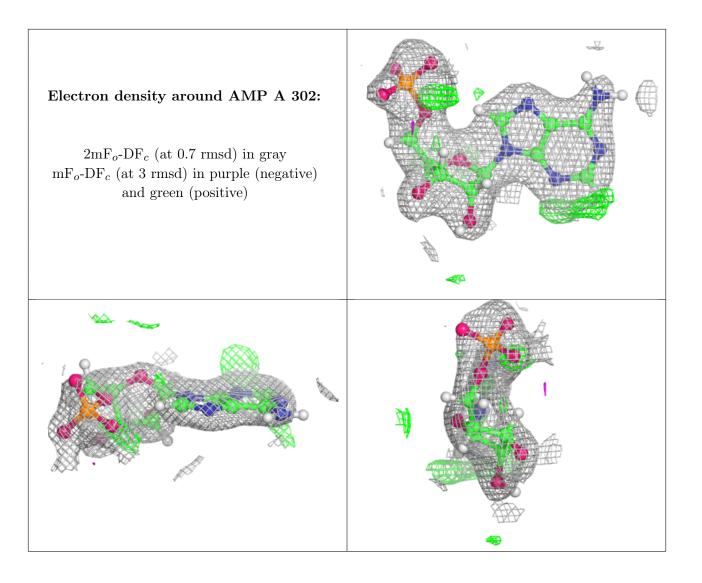
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
3	T7Q	D	302	21/21	0.79	0.17	$35,\!46,\!57,\!66$	34
7	PEG	А	303	7/7	0.88	0.20	51,61,72,82	0
4	MG	D	305	1/1	0.90	0.06	36,36,36,36	1
6	AMP	А	302	23/23	0.90	0.13	35,53,71,72	34
2	ATP	D	301	31/31	0.90	0.10	22,30,41,45	42
4	MG	D	303	1/1	0.95	0.09	24,24,24,24	1
5	GOL	А	301	6/6	0.95	0.21	23,29,52,52	0
4	MG	D	304	1/1	0.97	0.16	30,30,30,30	1

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.

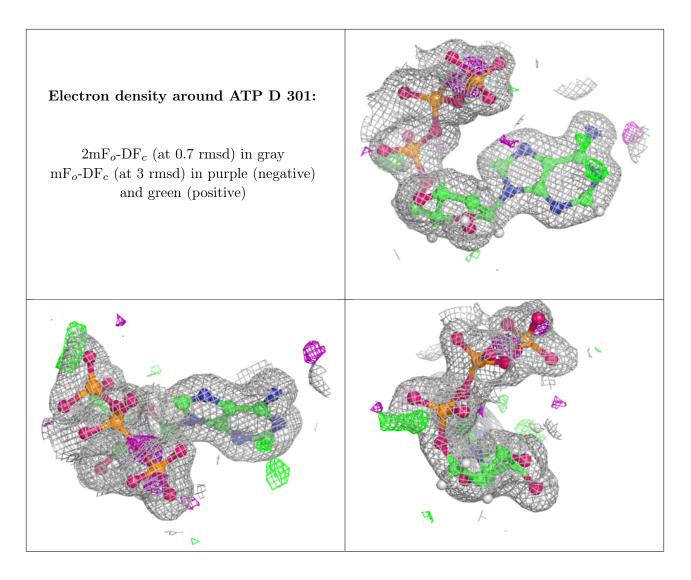












## 6.5 Other polymers (i)

There are no such residues in this entry.

