



# wwPDB X-ray Structure Validation Summary Report

Mar 5, 2026 – 09:01 PM UTC

PDB ID : 2DQS / pdb\_00002dqs  
Title : Crystal structure of the calcium pump with amppcp in the absence of calcium  
Authors : Toyoshima, C.; Norimatsu, Y.; Tsueda, J.  
Deposited on : 2006-05-29  
Resolution : 2.50 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

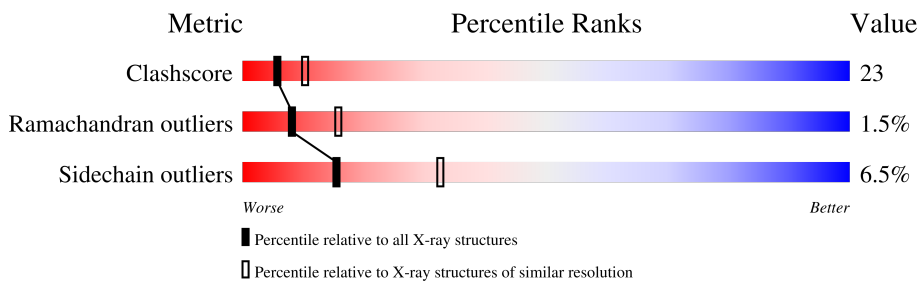
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	995	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8024 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 Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	995	7674	4878	1287	1452	57	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	-	SEE REMARK 999	UNP P04191

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

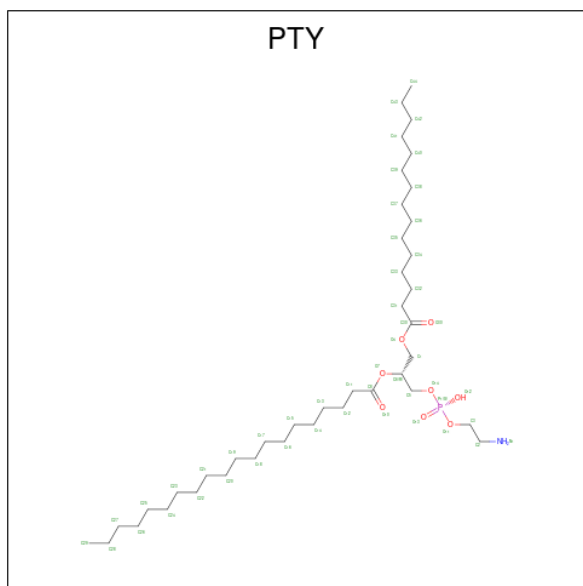
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



- Molecule 6 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		
6	A	1	Total	C	N	O	P	0	0
			19	9	1	8	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	232	Total	O	0	0
			232	232		



L959	D963	L964	T965	Q966	L968	M969	V970	I973	S974	L975	P976	V977	I978	G979	E982	I983	F986	I987	A988	R989	N990	G994
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.42Å 71.42Å 589.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 2.50	Depositor
% Data completeness (in resolution range)	98.8 (14.97-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.234 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

## 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: NA, TG1, MG, ACP, ACE, PTY

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	0.45	0/7813	0.95	20/10594 (0.2%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	VAL	CA-C-N	7.41	129.10	119.84
1	A	194	VAL	C-N-CA	7.41	129.10	119.84
1	A	683	HIS	N-CA-C	7.30	119.02	111.14
1	A	870	LEU	N-CA-C	-7.04	103.79	112.38
1	A	838	MET	N-CA-C	-6.51	103.87	110.97

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	A	7674	0	7765	365	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	31	0	14	1	0
5	A	46	0	50	2	0
6	A	38	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	232	0	0	7	0
All	All	8024	0	7851	365	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 23.

The worst 5 of 365 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:663:LEU:HD12	1:A:663:LEU:H	1.32	0.93
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.49	0.92
1:A:484:THR:HB	1:A:496:VAL:HG12	1.53	0.91
1:A:328:LYS:HA	1:A:328:LYS:NZ	1.85	0.90
1:A:739:ASN:HD22	1:A:740:PHE:N	1.72	0.87

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	993/995 (100%)	906 (91%)	72 (7%)	15 (2%)	<b>8</b> <b>16</b>

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	883	PHE
1	A	463	SER
1	A	861	ASP
1	A	951	ASP
1	A	132	ALA

### 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	A	840/840 (100%)	785 (94%)	55 (6%)	15 32

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	544	LYS
1	A	608	MET
1	A	990	ASN
1	A	872	HIS
1	A	562	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	ASN
1	A	919	ASN
1	A	666	GLN
1	A	966	GLN
1	A	880	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	TG1	A	1003	-	44,48,48	1.67	9 (20%)	47,72,72	1.80	11 (23%)
6	PTY	A	1012	-	18,18,49	1.12	3 (16%)	21,23,54	1.27	2 (9%)
4	ACP	A	1002	2	31,33,33	2.06	7 (22%)	47,52,52	1.73	6 (12%)
6	PTY	A	1011	-	18,18,49	1.19	3 (16%)	21,23,54	1.35	2 (9%)

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	TG1	A	1003	-	-	6/33/99/99	0/3/3/3
6	PTY	A	1012	-	-	10/20/20/53	-
4	ACP	A	1002	2	-	2/19/38/38	0/3/3/3
6	PTY	A	1011	-	-	9/20/20/53	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	ACP	PB-O3A	7.04	1.66	1.58
5	A	1003	TG1	O4-C21	4.67	1.31	1.21
5	A	1003	TG1	C3-C4	4.12	1.55	1.50
4	A	1002	ACP	PB-O2B	-3.98	1.46	1.56
4	A	1002	ACP	C5-N7	-3.21	1.33	1.39

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	ACP	C5'-C4'-C3'	-5.55	95.23	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	TG1	C10-O9-C32	5.51	134.28	121.36
4	A	1002	ACP	O5'-C5'-C4'	5.47	127.60	108.99
5	A	1003	TG1	C2-O1-C13	4.85	125.48	117.59
5	A	1003	TG1	O12-C12-C11	-4.27	123.96	128.28

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

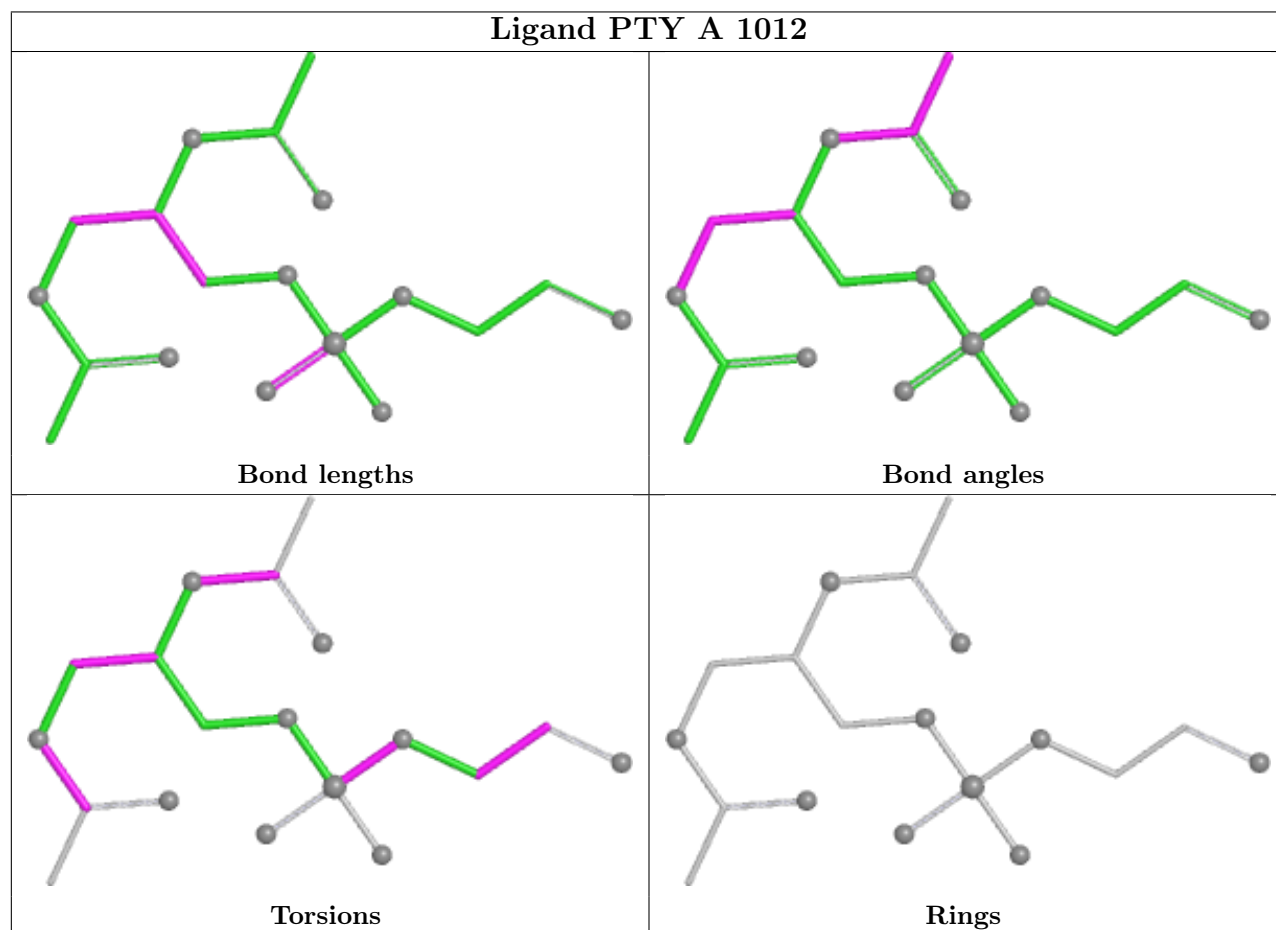
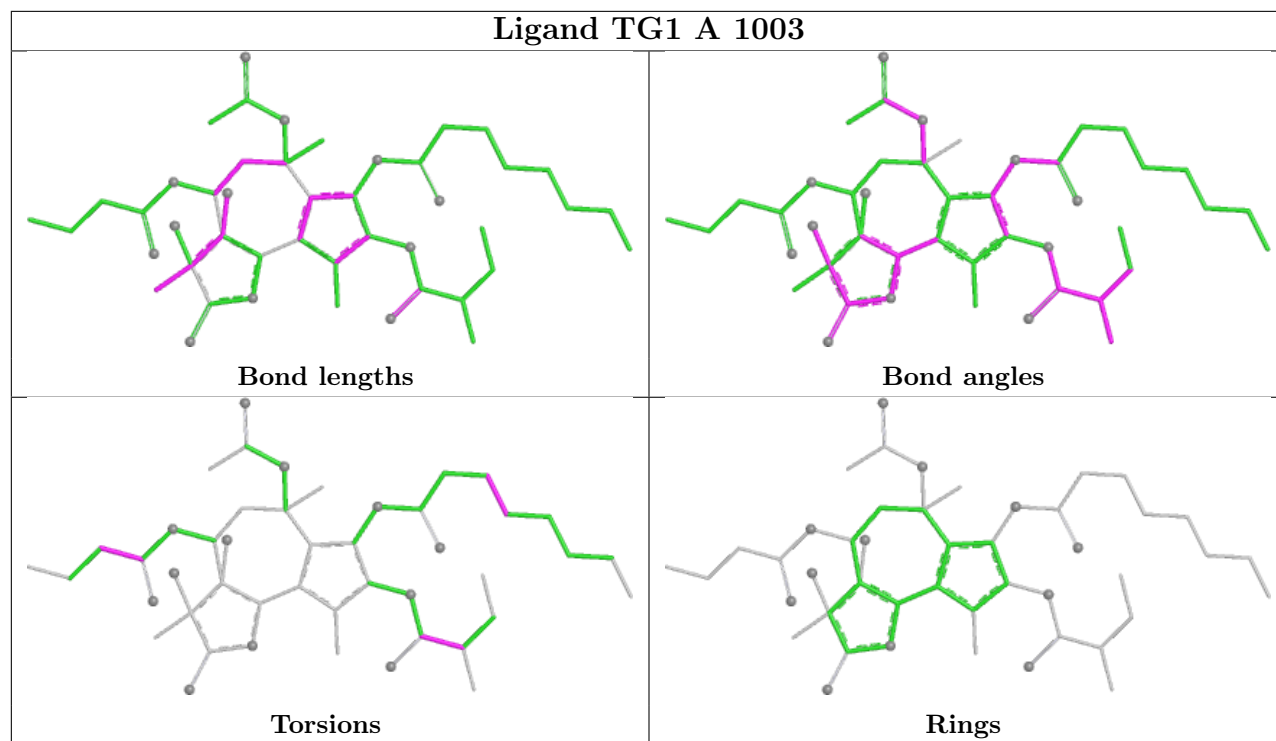
Mol	Chain	Res	Type	Atoms
5	A	1003	TG1	O3-C21-C22-C23
6	A	1011	PTY	N1-C2-C3-O11
6	A	1011	PTY	C11-C8-O7-C6
6	A	1012	PTY	N1-C2-C3-O11
6	A	1012	PTY	C11-C8-O7-C6

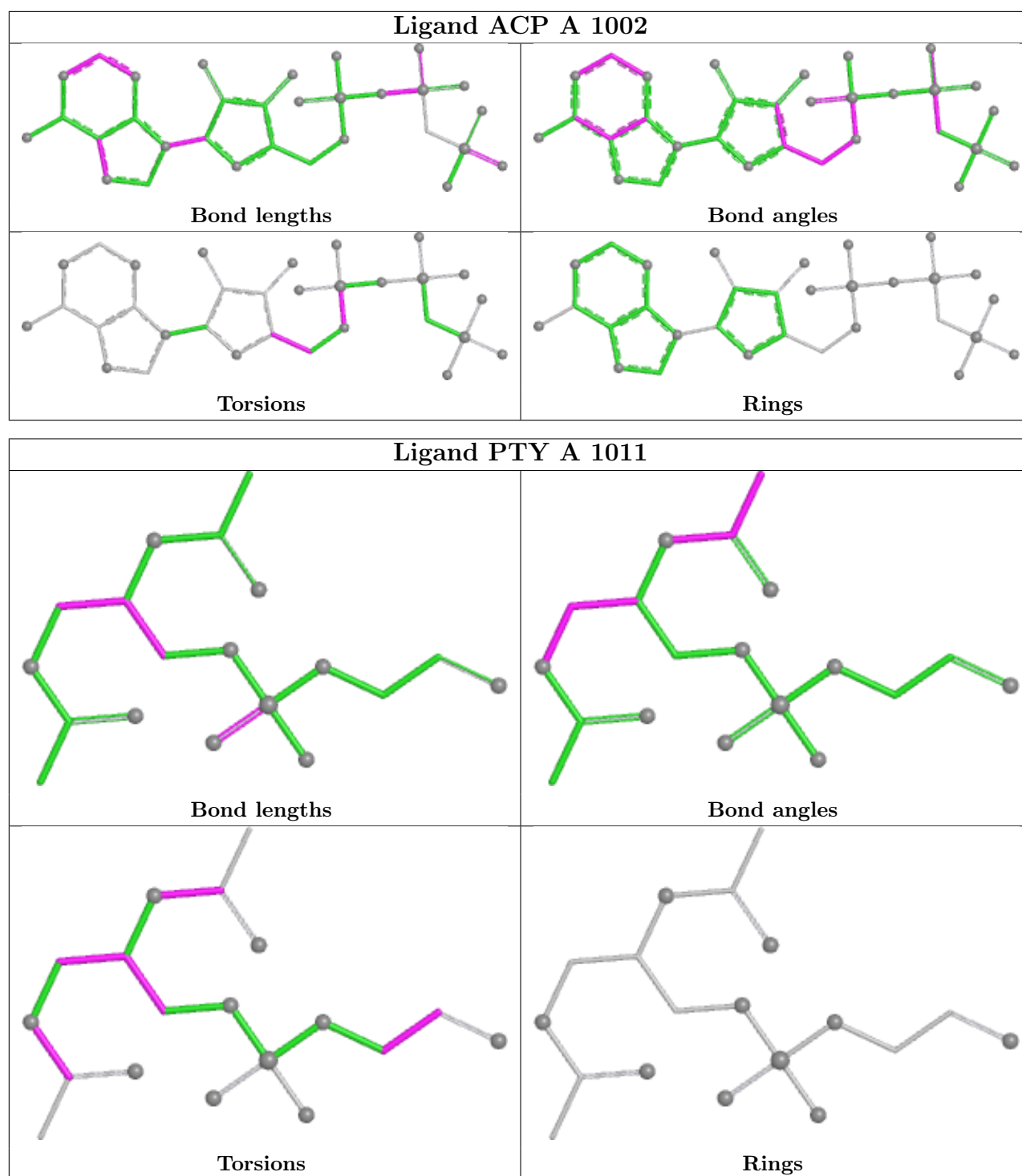
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1003	TG1	2	0
4	A	1002	ACP	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 than 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

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.