



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2022 – 08:18 PM EDT

PDB ID : 5E7P
Title : Crystal Structure of MSMEG_0858 (Uniprot A0QQS4), a AAA ATPase.
Authors : Unciulac-Carp, M.; Smith, P.; Shuman, S.
Deposited on : 2015-10-12
Resolution : 2.51 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 ⓘ symbol.

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

MolProbity : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

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 2.51 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

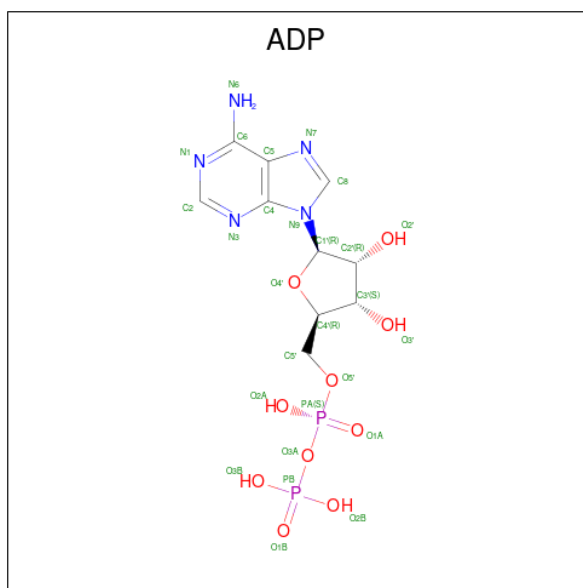
There are 6 unique types of molecules in this entry. The entry contains 10908 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cell division control protein Cdc48.

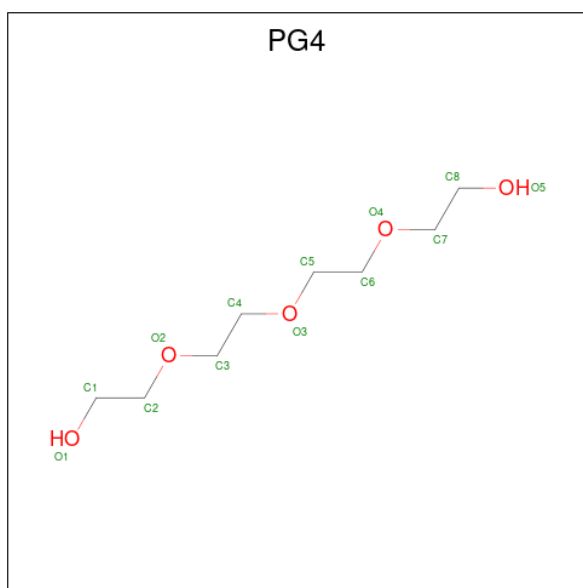
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	719	Total 5267	C 3284	N 943	O 1028	S 12	0	1	0
1	B	704	Total 5150	C 3209	N 917	O 1011	S 13	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



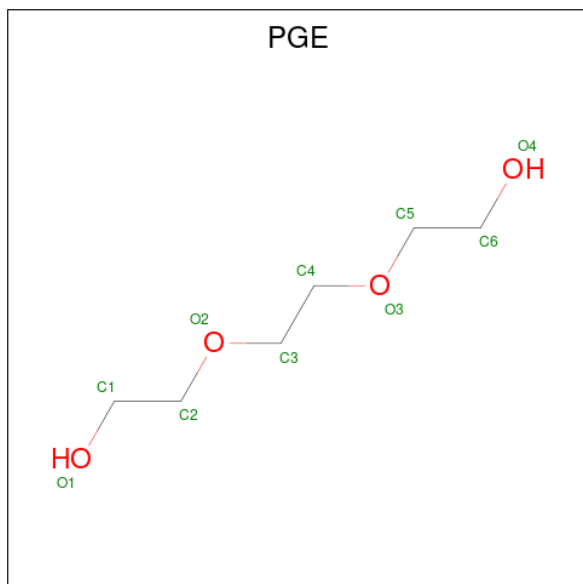
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	180	Total	O	0	0
			180	180		
6	B	152	Total	O	0	0
			152	152		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.80Å 111.82Å 151.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.52 – 2.51	Depositor
% Data completeness (in resolution range)	99.7 (29.52-2.51)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.51Å)	Xtrriage
Refinement program	PHENIX dev_833	Depositor
R, R_{free}	0.206 , 0.251	Depositor
Wilson B-factor (Å ²)	37.8	Xtrriage
Anisotropy	0.645	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10908	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9797e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

10 ligands 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
2	ADP	A	902	-	24,29,29	0.99	1 (4%)	29,45,45	1.35	4 (13%)
2	ADP	B	902	-	24,29,29	0.96	1 (4%)	29,45,45	1.30	4 (13%)
3	PG4	A	903	-	12,12,12	0.71	0	11,11,11	1.54	1 (9%)
4	GOL	A	905	-	5,5,5	0.36	0	5,5,5	0.32	0
4	GOL	B	905	-	5,5,5	0.38	0	5,5,5	0.16	0
5	PGE	B	903	-	9,9,9	0.67	0	8,8,8	1.49	1 (12%)
4	GOL	A	904	-	5,5,5	0.40	0	5,5,5	0.25	0
2	ADP	B	901	-	24,29,29	0.97	1 (4%)	29,45,45	1.38	4 (13%)
2	ADP	A	901	-	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)
5	PGE	B	904	-	9,9,9	0.67	0	8,8,8	1.65	1 (12%)

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
2	ADP	A	902	-	-	4/12/32/32	0/3/3/3
2	ADP	B	902	-	-	3/12/32/32	0/3/3/3
3	PG4	A	903	-	-	6/10/10/10	-
4	GOL	A	905	-	-	4/4/4/4	-
4	GOL	B	905	-	-	2/4/4/4	-
5	PGE	B	903	-	-	2/7/7/7	-
4	GOL	A	904	-	-	4/4/4/4	-
2	ADP	B	901	-	-	3/12/32/32	0/3/3/3
2	ADP	A	901	-	-	4/12/32/32	0/3/3/3
5	PGE	B	904	-	-	5/7/7/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	ADP	C5-C4	2.54	1.47	1.40
2	B	901	ADP	C5-C4	2.49	1.47	1.40
2	B	902	ADP	C5-C4	2.43	1.47	1.40
2	A	901	ADP	C5-C4	2.39	1.47	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	ADP	C3'-C2'-C1'	3.52	106.28	100.98
2	A	901	ADP	N3-C2-N1	-3.47	123.26	128.68
2	B	901	ADP	PA-O3A-PB	-3.19	121.87	132.83
2	B	902	ADP	C3'-C2'-C1'	3.15	105.72	100.98
2	B	901	ADP	N3-C2-N1	-3.12	123.81	128.68
2	B	902	ADP	N3-C2-N1	-3.06	123.90	128.68
2	A	901	ADP	PA-O3A-PB	-3.00	122.54	132.83
2	A	902	ADP	N3-C2-N1	-2.93	124.09	128.68
2	A	901	ADP	C3'-C2'-C1'	2.80	105.20	100.98
2	B	901	ADP	C3'-C2'-C1'	2.73	105.09	100.98
2	A	901	ADP	C4-C5-N7	-2.72	106.56	109.40
2	B	901	ADP	C4-C5-N7	-2.72	106.56	109.40
3	A	903	PG4	O2-C2-C1	2.67	121.82	110.07
2	B	902	ADP	C4-C5-N7	-2.65	106.64	109.40
2	A	902	ADP	C4-C5-N7	-2.58	106.71	109.40
5	B	904	PGE	O2-C2-C1	2.31	120.22	110.07
2	A	902	ADP	PA-O3A-PB	-2.25	125.09	132.83
5	B	903	PGE	O3-C4-C3	2.08	119.75	110.39
2	B	902	ADP	PA-O3A-PB	-2.06	125.77	132.83

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ADP	PA-O3A-PB-O2B
2	A	902	ADP	O4'-C4'-C5'-O5'
2	A	902	ADP	C3'-C4'-C5'-O5'
2	B	901	ADP	PA-O3A-PB-O3B
2	B	902	ADP	PA-O3A-PB-O2B
4	A	904	GOL	O1-C1-C2-O2
4	A	904	GOL	O1-C1-C2-C3
4	A	904	GOL	C1-C2-C3-O3
4	A	905	GOL	O1-C1-C2-C3
2	B	902	ADP	O4'-C4'-C5'-O5'
3	A	903	PG4	O2-C3-C4-O3
5	B	904	PGE	O2-C3-C4-O3
3	A	903	PG4	O4-C7-C8-O5
2	B	902	ADP	C3'-C4'-C5'-O5'
4	A	905	GOL	C1-C2-C3-O3
4	B	905	GOL	C1-C2-C3-O3
4	A	904	GOL	O2-C2-C3-O3

Continued on next page...

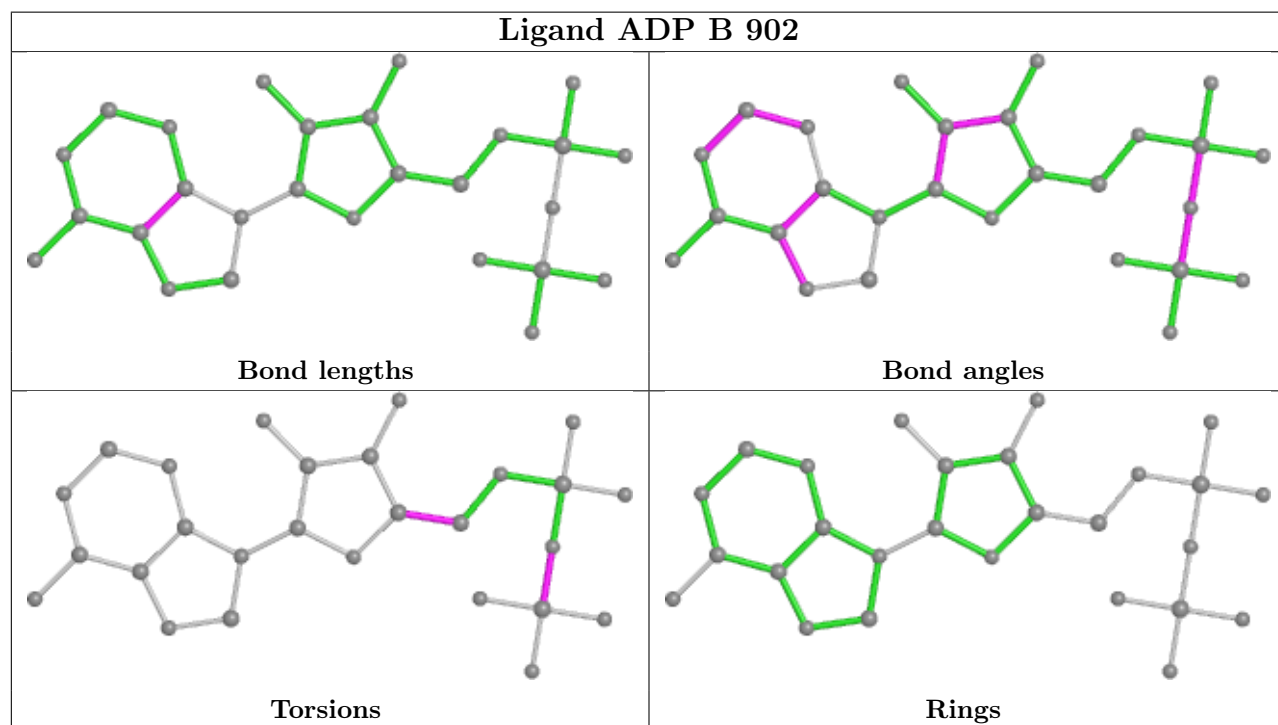
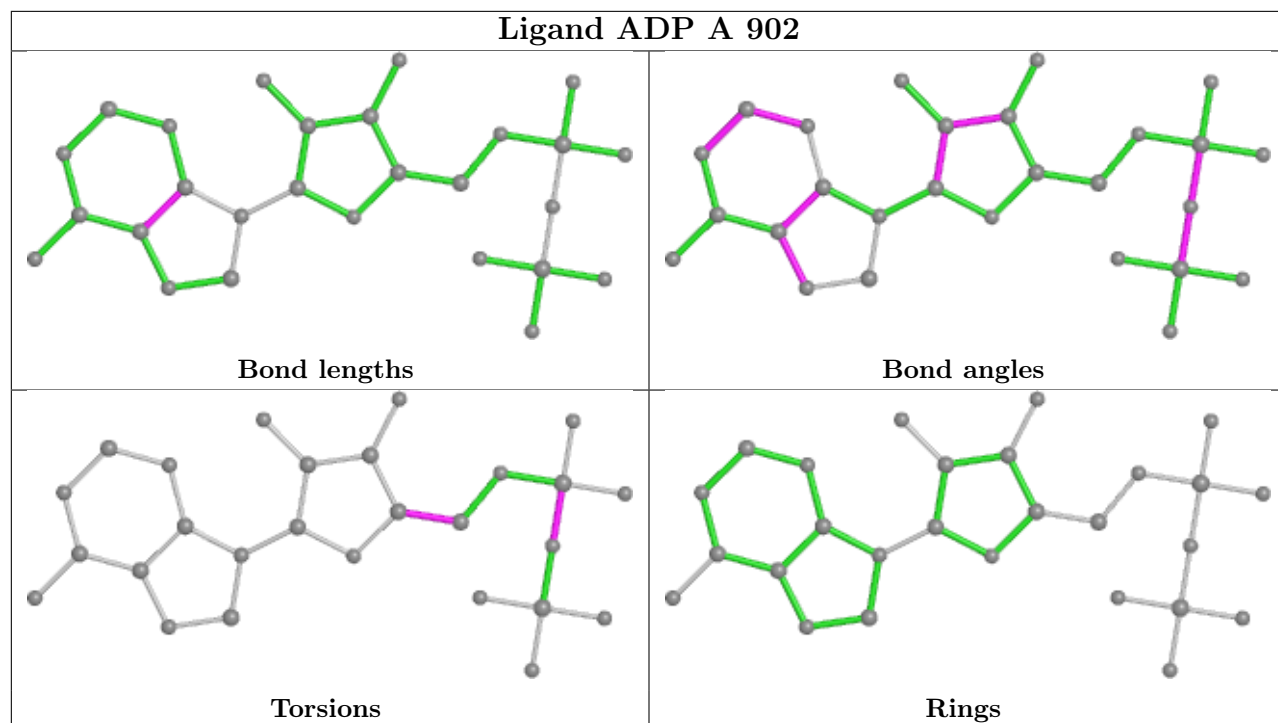
Continued from previous page...

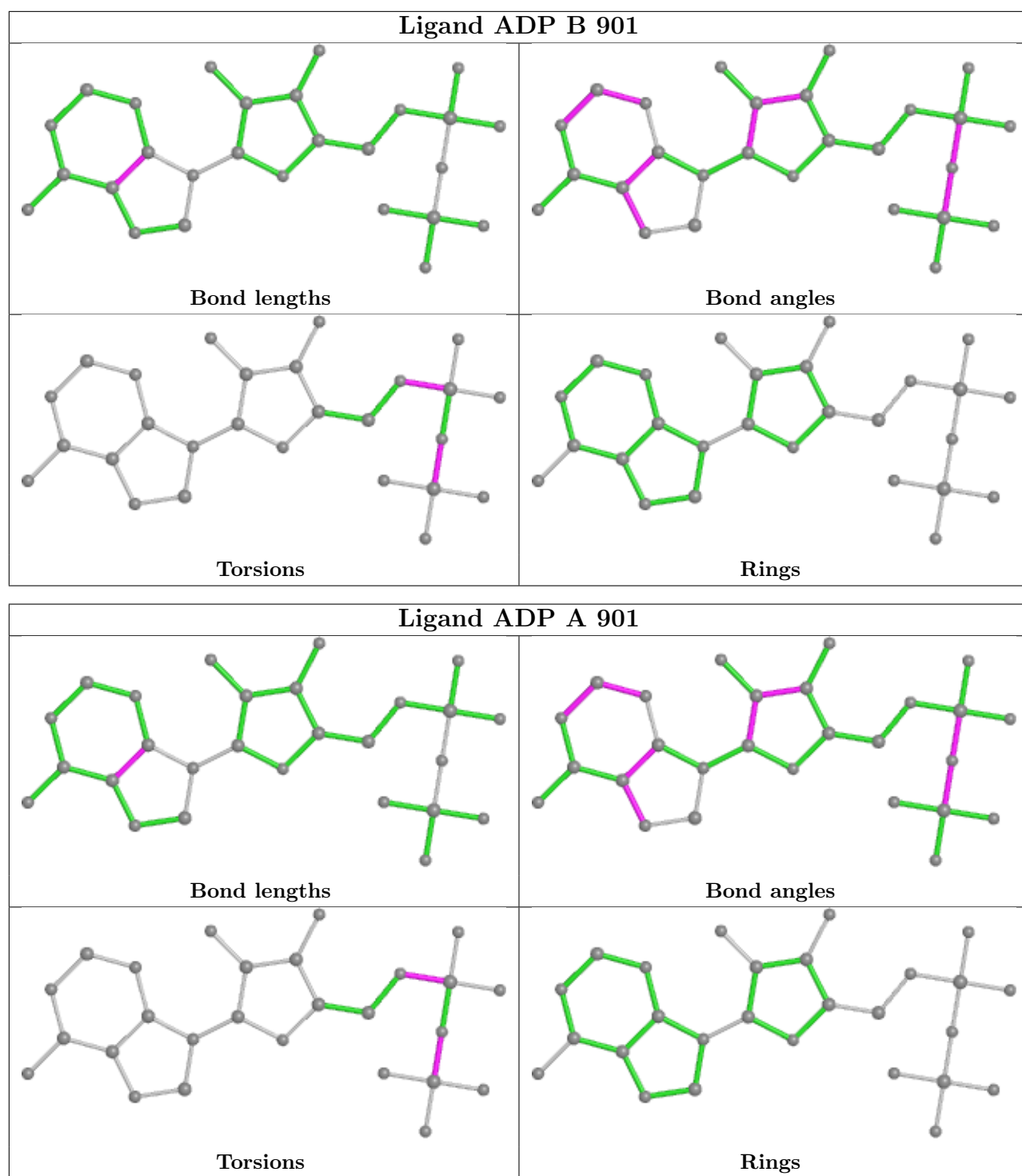
Mol	Chain	Res	Type	Atoms
4	A	905	GOL	O1-C1-C2-O2
4	B	905	GOL	O2-C2-C3-O3
5	B	903	PGE	O3-C5-C6-O4
2	A	901	ADP	C5'-O5'-PA-O3A
2	B	901	ADP	C5'-O5'-PA-O3A
2	A	902	ADP	PB-O3A-PA-O1A
5	B	904	PGE	C1-C2-O2-C3
5	B	904	PGE	C6-C5-O3-C4
3	A	903	PG4	C8-C7-O4-C6
4	A	905	GOL	O2-C2-C3-O3
3	A	903	PG4	C5-C6-O4-C7
3	A	903	PG4	C3-C4-O3-C5
3	A	903	PG4	O3-C5-C6-O4
2	A	901	ADP	PA-O3A-PB-O1B
2	B	901	ADP	PA-O3A-PB-O1B
5	B	904	PGE	C4-C3-O2-C2
5	B	903	PGE	O2-C3-C4-O3
2	A	902	ADP	PB-O3A-PA-O2A
2	A	901	ADP	C5'-O5'-PA-O1A
5	B	904	PGE	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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.





4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.