



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2022 – 08:02 PM EDT

PDB ID : 5V0V  
Title : Crystal structure of Equine Serum Albumin complex with etodolac  
Authors : Czub, M.P.; Shabalin, I.G.; Handing, K.B.; Venkataramany, B.S.; Steen, E.H.; Anderson, W.F.; Minor, W.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2017-02-28  
Resolution : 2.45 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](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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	<b>FAILED</b>
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	<b>FAILED</b>
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 2.45 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.

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
2	TRS	A	604	-	X	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4827 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.

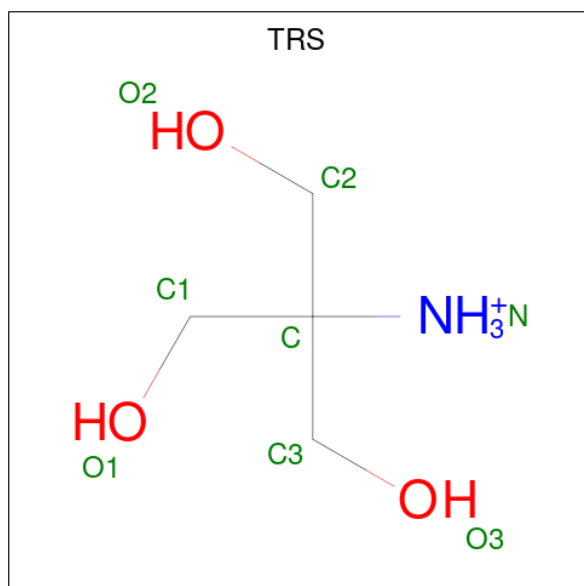
- Molecule 1 is a protein called Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	581	4512	2859	751	867	35	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	ALA	ARG	conflict	UNP P35747

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	4	1	3	0	0
2	A	1	8	4	1	3	0	0

*Continued on next page...*

Continued from previous page...

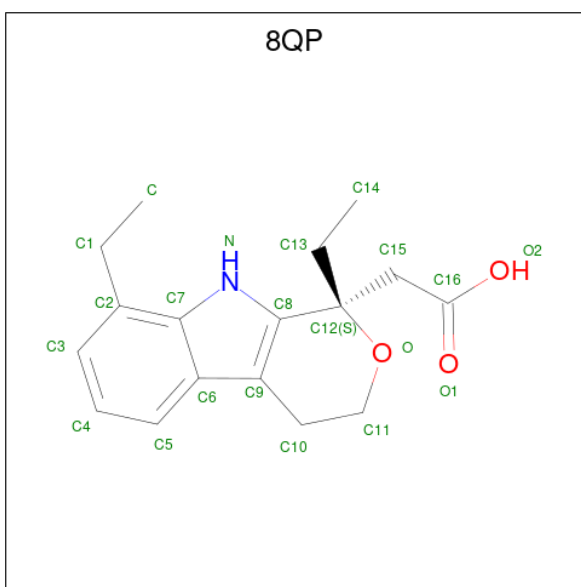
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



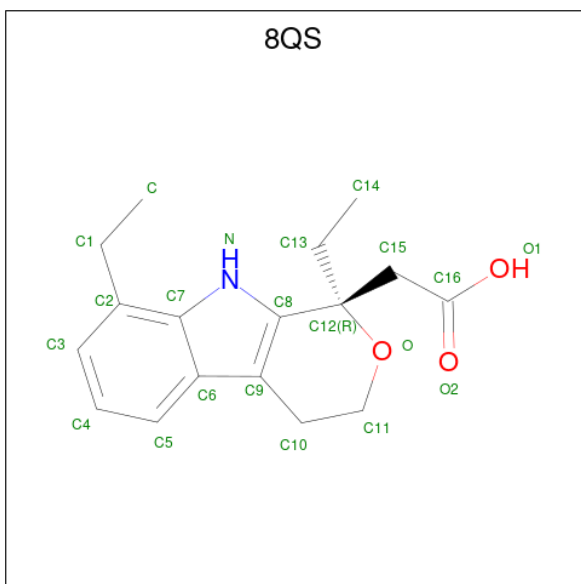
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is [(1S)-1,8-diethyl-1,3,4,9-tetrahydropyrano[3,4-b]indol-1-yl]acetic acid (three-letter code: 8QP) (formula: C<sub>17</sub>H<sub>21</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	17	1	3		
4	A	1	Total	C	N	O	0	0
			21	17	1	3		

- Molecule 5 is [(1R)-1,8-diethyl-1,3,4,9-tetrahydropyrano[3,4-b]indol-1-yl]acetic acid (three-letter code: 8QS) (formula: C<sub>17</sub>H<sub>21</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	17	1	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			21	17	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	164	Total	O	0	0
			164	164		

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 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.21Å 94.21Å 141.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.45	Depositor
% Data completeness (in resolution range)	99.9 (50.00-2.45)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.180 , 0.238	Depositor
Wilson B-factor (Å <sup>2</sup> )	51.0	Xtriage
Anisotropy	0.401	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.060 for h,-h-k,-l	Xtriage
Total number of atoms	4827	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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, 0.333 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](#)

15 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	$\# Z  > 2$
3	SO4	A	606	-	4,4,4	0.30	0	6,6,6	0.11	0
3	SO4	A	608	-	4,4,4	0.34	0	6,6,6	0.05	0
3	SO4	A	609	-	4,4,4	0.34	0	6,6,6	0.08	0
5	8QS	A	615	-	16,23,23	0.84	0	13,34,34	1.44	2 (15%)
2	TRS	A	602	-	7,7,7	0.40	0	9,9,9	0.65	0
3	SO4	A	607	-	4,4,4	0.32	0	6,6,6	0.07	0
5	8QS	A	614	-	16,23,23	0.82	0	13,34,34	0.82	0
3	SO4	A	605	-	4,4,4	0.34	0	6,6,6	0.07	0
3	SO4	A	610	-	4,4,4	0.34	0	6,6,6	0.12	0
2	TRS	A	603	-	7,7,7	0.42	0	9,9,9	0.49	0
4	8QP	A	613	-	16,23,23	0.82	0	13,34,34	1.53	1 (7%)
2	TRS	A	601	-	7,7,7	0.42	0	9,9,9	0.75	0
2	TRS	A	604	-	7,7,7	0.59	0	9,9,9	1.09	1 (11%)
3	SO4	A	611	-	4,4,4	0.35	0	6,6,6	0.06	0
4	8QP	A	612	-	16,23,23	0.77	0	13,34,34	1.28	1 (7%)

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	8QS	A	615	-	-	1/8/23/23	0/3/3/3
2	TRS	A	602	-	-	6/9/9/9	-
5	8QS	A	614	-	-	1/8/23/23	0/3/3/3
2	TRS	A	603	-	-	3/9/9/9	-
4	8QP	A	613	-	-	2/8/23/23	0/3/3/3
2	TRS	A	601	-	-	9/9/9/9	-
2	TRS	A	604	-	-	9/9/9/9	-
4	8QP	A	612	-	-	1/8/23/23	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	613	8QP	C11-C10-C9	-5.18	103.13	110.82

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	615	8QS	C11-C10-C9	-4.01	104.87	110.82
4	A	612	8QP	O-C11-C10	4.00	117.52	110.65
2	A	604	TRS	O3-C3-C	2.55	119.08	111.00
5	A	615	8QS	O-C11-C10	2.52	114.97	110.65

There are no chirality outliers.

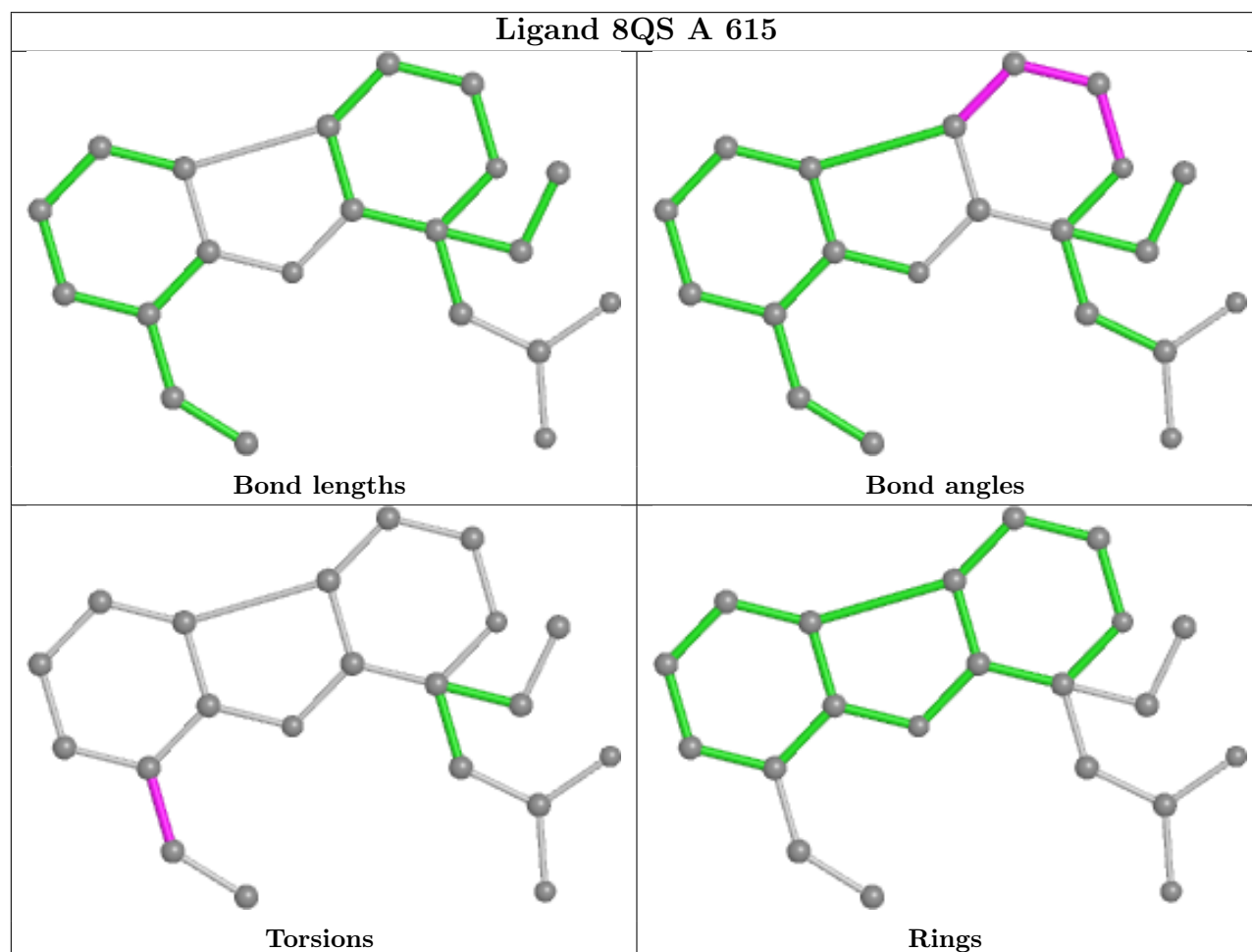
All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	TRS	N-C-C3-O3
2	A	602	TRS	C1-C-C2-O2
2	A	604	TRS	C2-C-C1-O1
2	A	604	TRS	C3-C-C1-O1
2	A	604	TRS	N-C-C1-O1
2	A	604	TRS	C1-C-C2-O2
2	A	604	TRS	C3-C-C2-O2
2	A	604	TRS	C1-C-C3-O3
2	A	604	TRS	C2-C-C3-O3
2	A	604	TRS	N-C-C3-O3
5	A	614	8QS	C-C1-C2-C7
4	A	613	8QP	C-C1-C2-C3
2	A	601	TRS	C3-C-C1-O1
2	A	601	TRS	C1-C-C3-O3
2	A	601	TRS	N-C-C1-O1
2	A	601	TRS	C3-C-C2-O2
2	A	601	TRS	N-C-C2-O2
2	A	601	TRS	C2-C-C3-O3
2	A	602	TRS	C3-C-C1-O1
2	A	602	TRS	N-C-C1-O1
2	A	602	TRS	C3-C-C2-O2
2	A	603	TRS	C3-C-C2-O2
2	A	603	TRS	N-C-C2-O2
2	A	604	TRS	N-C-C2-O2
4	A	613	8QP	O-C12-C15-C16
4	A	612	8QP	C15-C12-C13-C14
5	A	615	8QS	C-C1-C2-C7
2	A	601	TRS	C2-C-C1-O1
2	A	602	TRS	C2-C-C1-O1
2	A	603	TRS	C1-C-C2-O2
2	A	601	TRS	C1-C-C2-O2
2	A	602	TRS	N-C-C2-O2

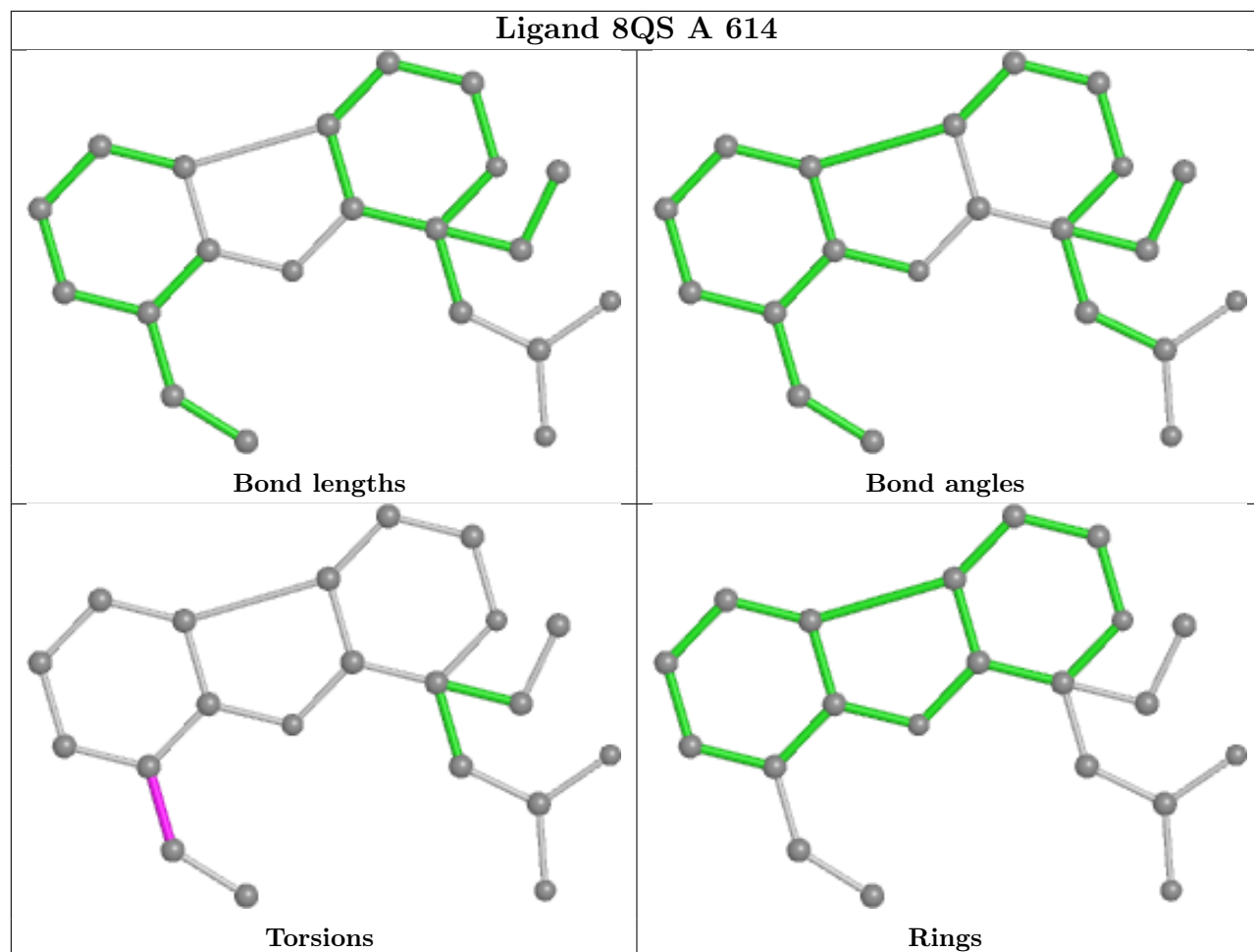
There are no ring outliers.

No monomer is involved in short contacts.

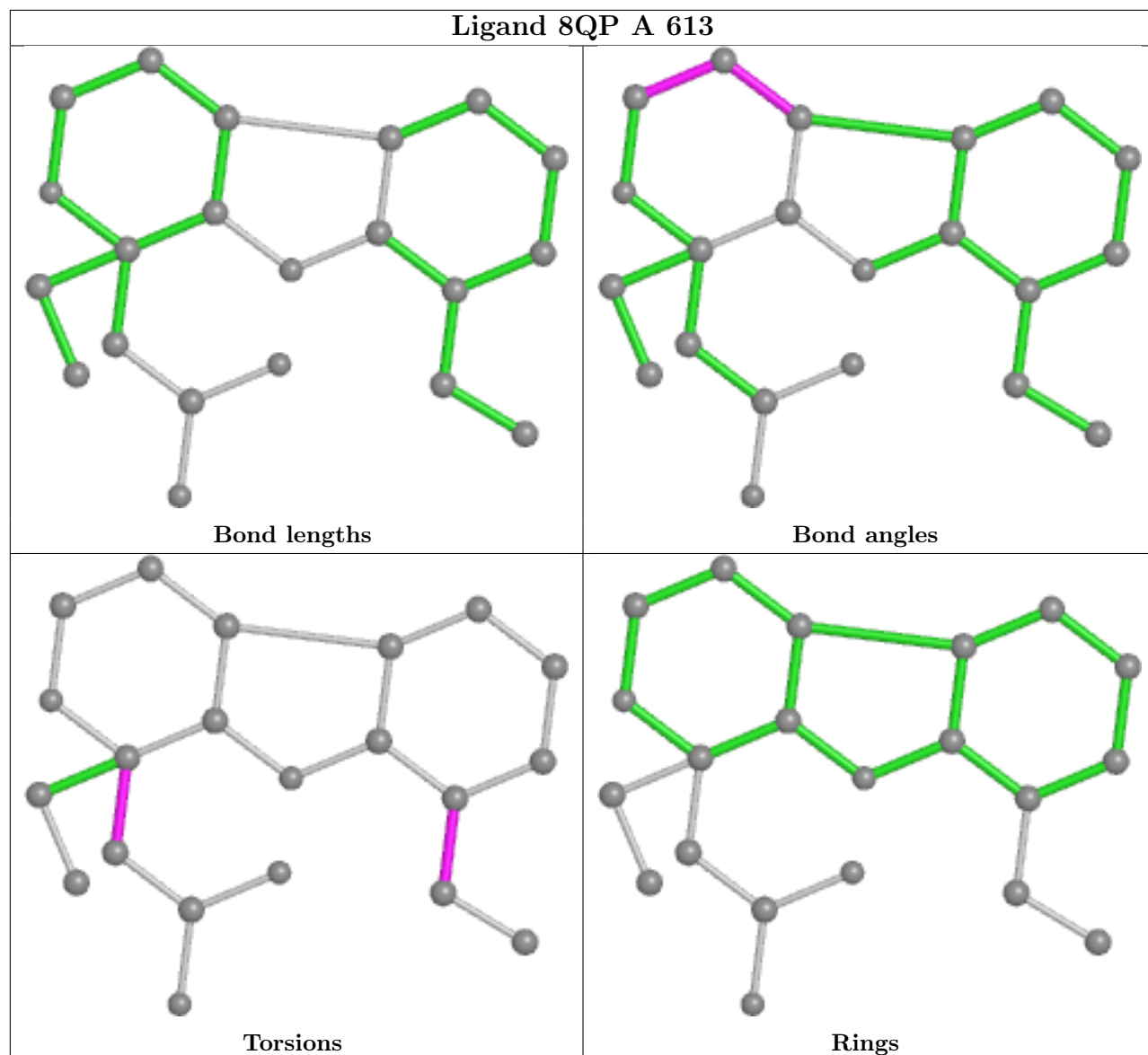
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

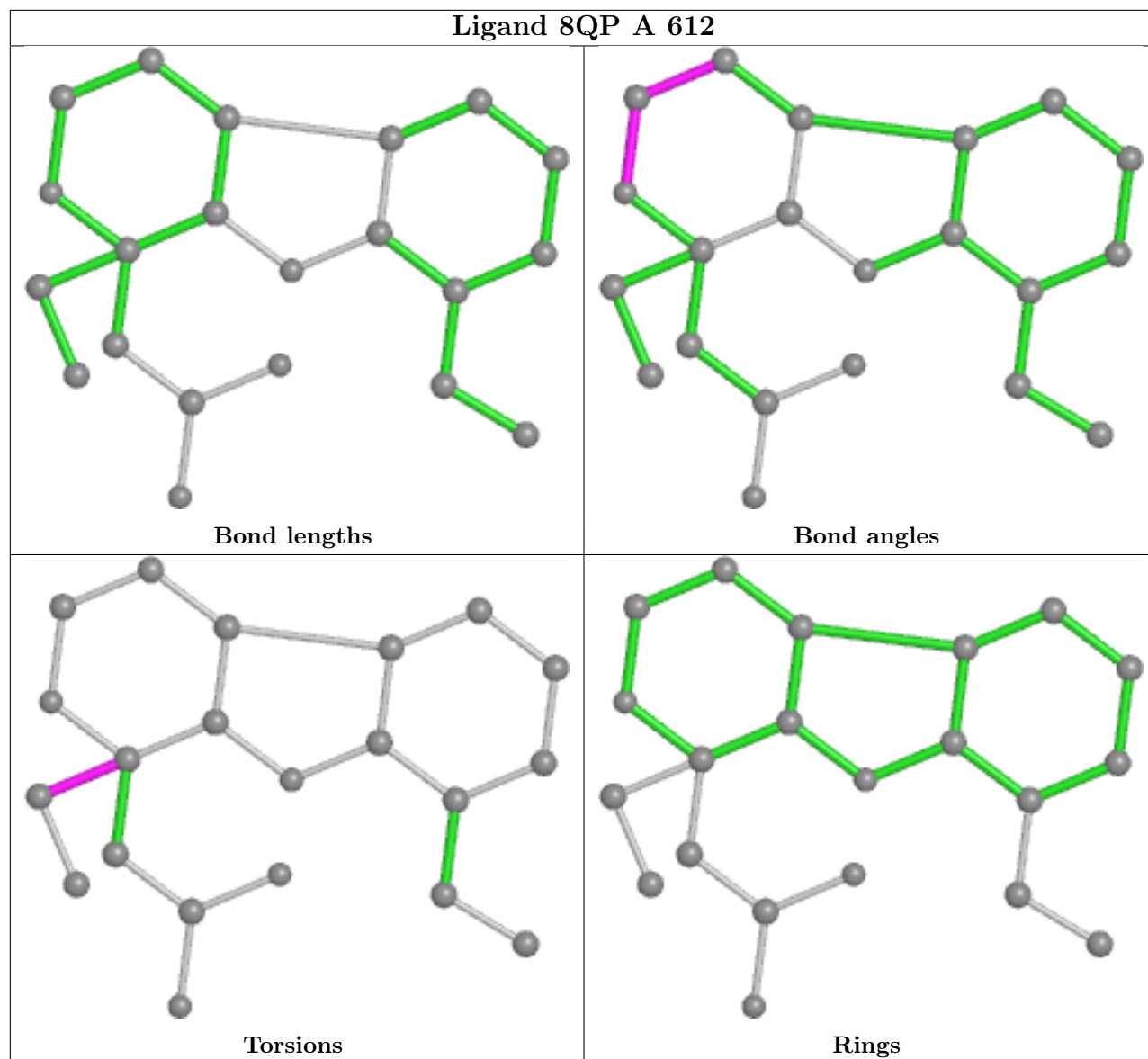


## Ligand 8QS A 614



## Ligand 8QP A 613





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

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

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.