



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 27, 2026 – 07:20 PM EDT

PDB ID : 6QCE / pdb_00006qce
Title : Human Sirt6 in complex with ADP-ribose and the activator isoquercetin
Authors : You, W.; Steegborn, C.
Deposited on : 2018-12-27
Resolution : 1.90 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
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 1.90 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

There are 7 unique types of molecules in this entry. The entry contains 4806 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.

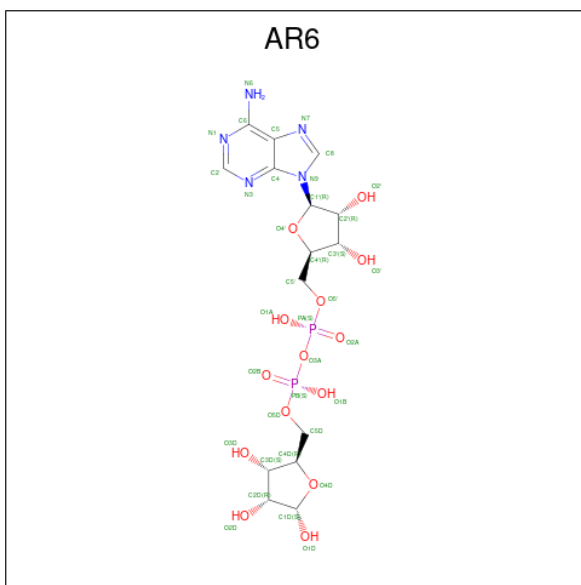
- Molecule 1 is a protein called NAD-dependent protein deacetylase sirtuin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	1	0
			2201	1386	400	403	12			
1	B	277	Total	C	N	O	S	0	3	0
			2180	1373	399	395	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	GLY	-	expression tag	UNP Q8N6T7
A	8	ILE	-	expression tag	UNP Q8N6T7
A	9	ASP	-	expression tag	UNP Q8N6T7
A	10	PRO	-	expression tag	UNP Q8N6T7
A	11	PHE	-	expression tag	UNP Q8N6T7
A	12	THR	-	expression tag	UNP Q8N6T7
B	7	GLY	-	expression tag	UNP Q8N6T7
B	8	ILE	-	expression tag	UNP Q8N6T7
B	9	ASP	-	expression tag	UNP Q8N6T7
B	10	PRO	-	expression tag	UNP Q8N6T7
B	11	PHE	-	expression tag	UNP Q8N6T7
B	12	THR	-	expression tag	UNP Q8N6T7

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	B	1	Total 36	C 15	N 5	O 14	P 2	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

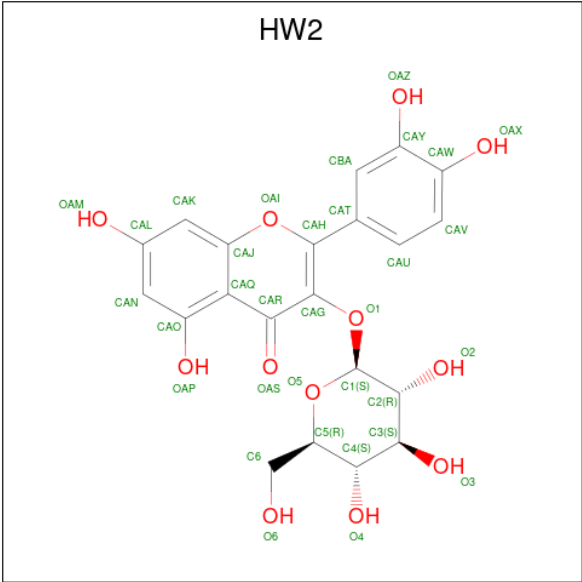
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



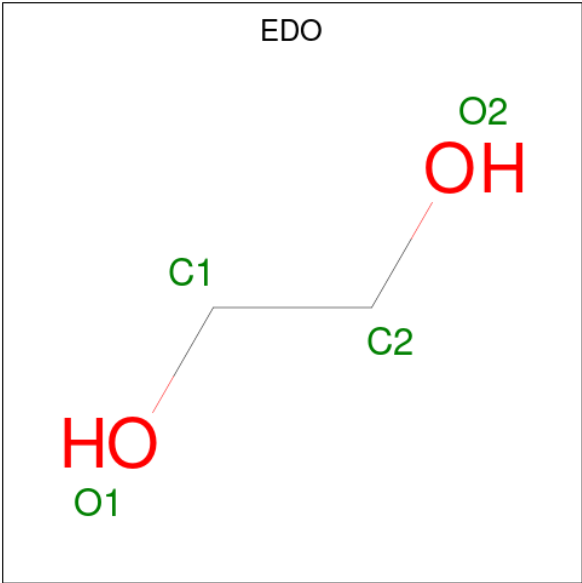
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is isoquercetin (CCD ID: HW2) (formula: C₂₁H₂₀O₁₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			33	21	12		
5	B	1	Total	C	O	0	0
			33	21	12		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	124	Total	O	0	0
			124	124		
7	B	100	Total	O	0	0
			100	100		

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 63	Depositor
Cell constants a, b, c, α , β , γ	91.41Å 91.41Å 144.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.57 – 1.90	Depositor
% Data completeness (in resolution range)	99.9 (43.57-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.152 , 0.187	Depositor
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.446	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.278 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.276 for H, K, L 0.724 for -K, -H, -L	Depositor
Outliers	0 of 53635 reflections	Xtriage
Total number of atoms	4806	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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 oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\# Z > 2$
6	EDO	A	411	-	3,3,3	0.42	0	2,2,2	0.38	0
4	SO4	B	406	-	4,4,4	0.31	0	6,6,6	0.12	0
5	HW2	B	407	-	36,36,36	1.98	10 (27%)	54,54,54	1.88	16 (29%)
4	SO4	A	405	-	4,4,4	0.35	0	6,6,6	0.06	0
5	HW2	A	408	-	36,36,36	1.73	7 (19%)	54,54,54	1.93	16 (29%)
6	EDO	A	410	-	3,3,3	0.09	0	2,2,2	0.14	0
4	SO4	A	404	-	4,4,4	0.39	0	6,6,6	0.08	0
2	AR6	A	401	-	39,39,39	1.86	3 (7%)	56,60,60	0.93	2 (3%)
4	SO4	A	407	-	4,4,4	0.24	0	6,6,6	0.11	0
6	EDO	A	412	-	3,3,3	0.18	0	2,2,2	0.03	0
4	SO4	A	403	-	4,4,4	0.43	0	6,6,6	0.18	0
2	AR6	B	401	-	39,39,39	0.84	2 (5%)	56,60,60	0.99	3 (5%)
6	EDO	A	409	-	3,3,3	0.17	0	2,2,2	0.17	0
4	SO4	B	404	-	4,4,4	0.33	0	6,6,6	0.18	0
4	SO4	A	406	-	4,4,4	0.32	0	6,6,6	0.10	0
4	SO4	B	403	-	4,4,4	0.66	0	6,6,6	0.45	0
4	SO4	B	405	-	4,4,4	0.30	0	6,6,6	0.13	0

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
6	EDO	A	411	-	-	0/1/1/1	-
5	HW2	B	407	-	-	6/10/30/30	0/4/4/4
5	HW2	A	408	-	-	6/10/30/30	0/4/4/4
6	EDO	A	410	-	-	0/1/1/1	-
6	EDO	A	412	-	-	1/1/1/1	-
2	AR6	A	401	-	-	2/22/54/54	0/4/4/4
2	AR6	B	401	-	-	1/22/54/54	0/4/4/4
6	EDO	A	409	-	-	1/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	AR6	PB-O3A	9.01	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	407	HW2	O1-C1	6.65	1.55	1.43
5	A	408	HW2	O1-C1	6.04	1.54	1.43
2	A	401	AR6	PA-O3A	5.61	1.65	1.59
5	B	407	HW2	CAT-CAH	-4.00	1.41	1.47

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	408	HW2	OAI-CAH-CAG	-4.68	114.54	120.44
5	B	407	HW2	C1-O1-CAG	-4.20	106.11	115.60
5	A	408	HW2	O5-C5-C6	4.18	116.80	106.44
5	A	408	HW2	OAI-CAJ-CAK	4.16	121.73	115.83
5	A	408	HW2	OAI-CAH-CAT	4.16	116.69	110.87

There are no chirality outliers.

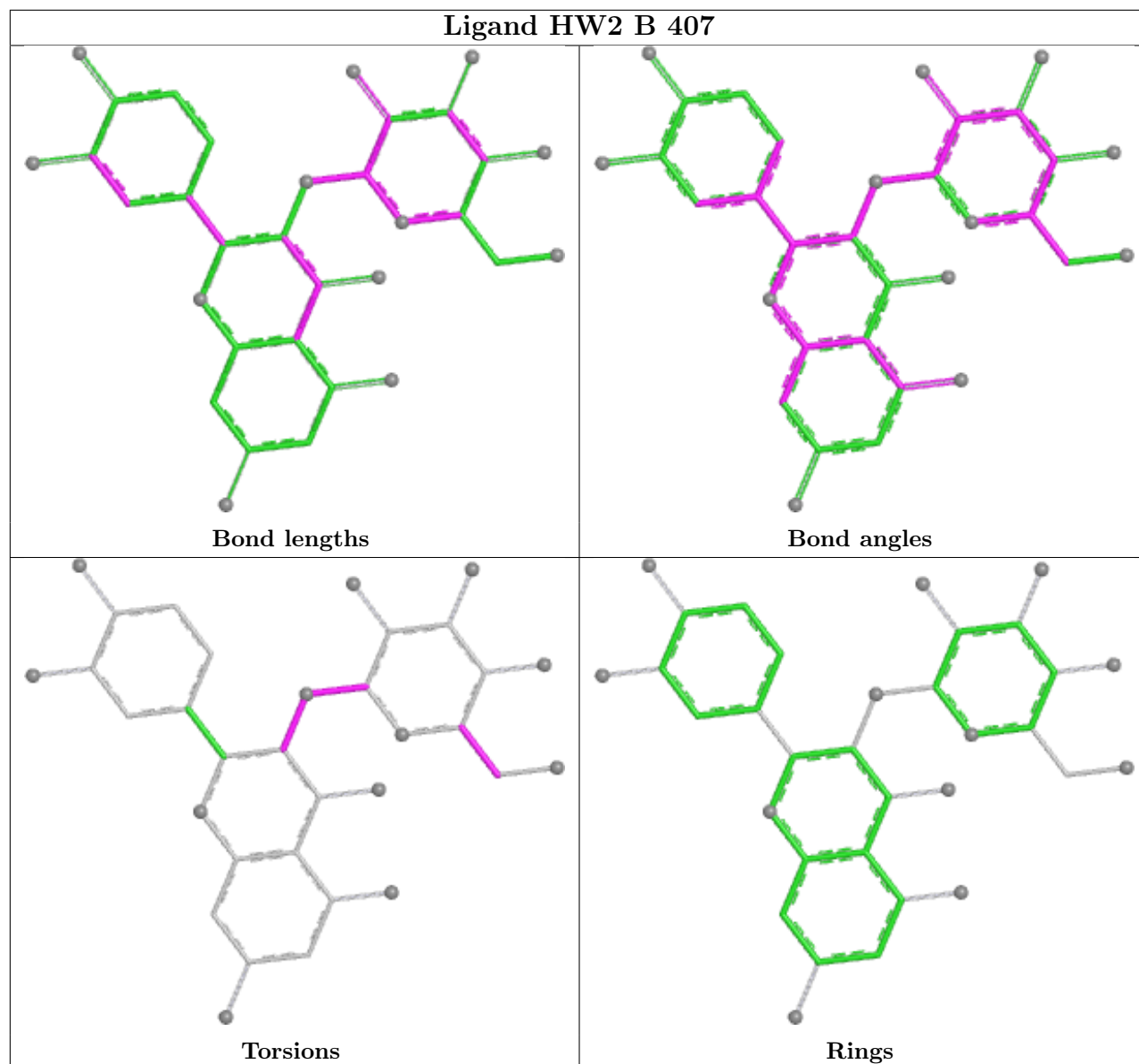
5 of 17 torsion outliers are listed below:

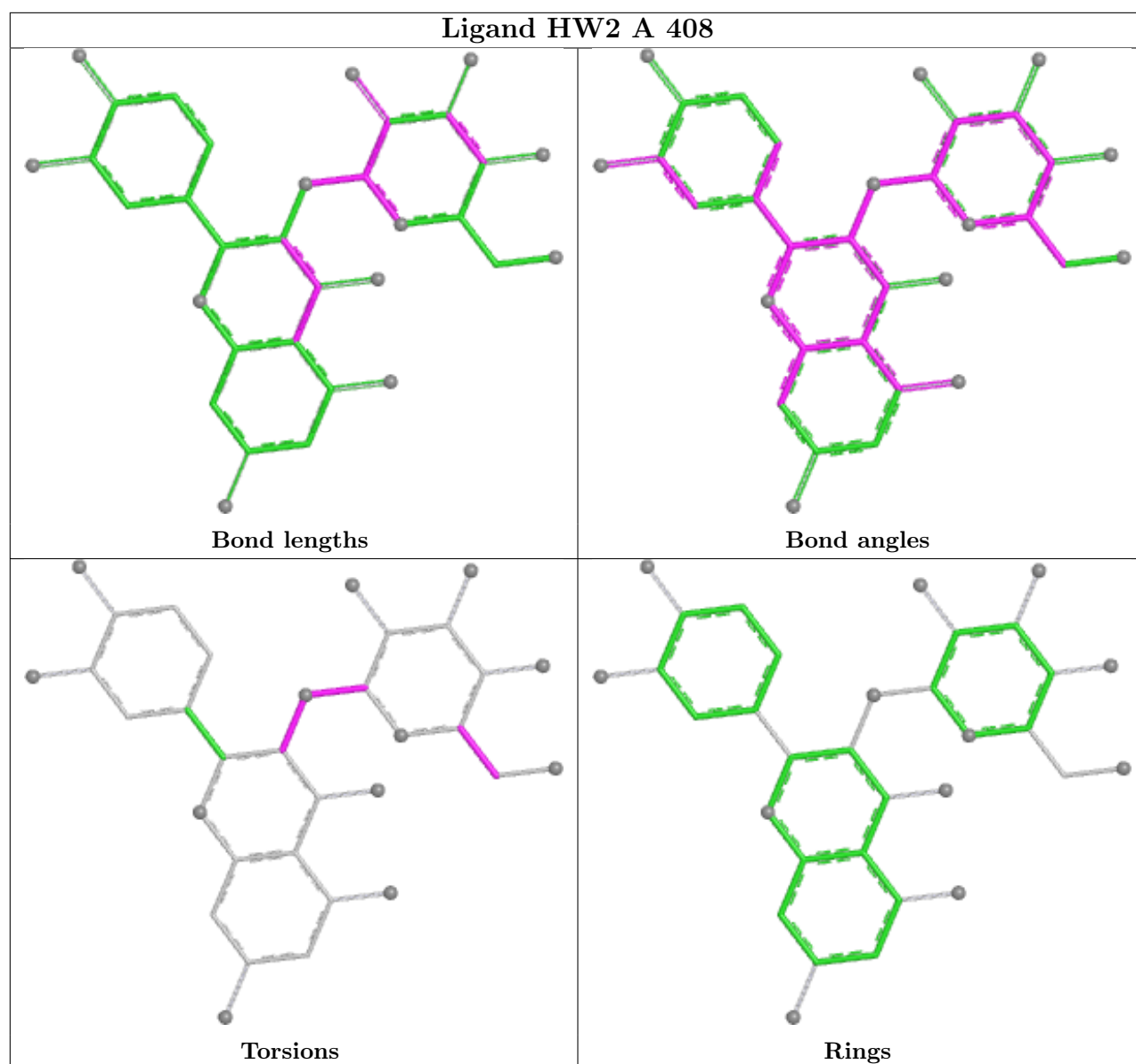
Mol	Chain	Res	Type	Atoms
5	A	408	HW2	CAR-CAG-O1-C1
5	A	408	HW2	O5-C1-O1-CAG
5	A	408	HW2	C2-C1-O1-CAG
5	B	407	HW2	O5-C1-O1-CAG
5	B	407	HW2	C2-C1-O1-CAG

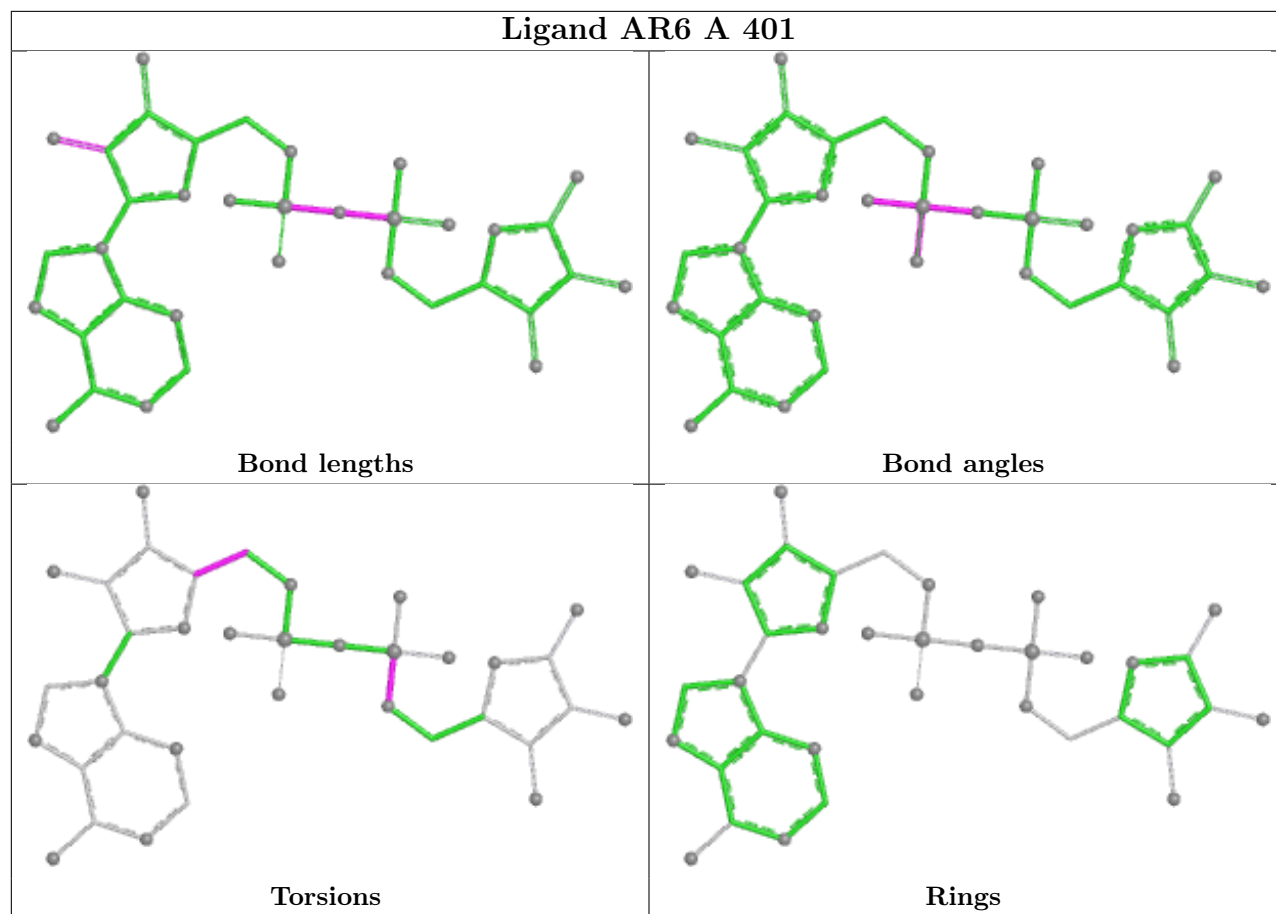
There are no ring outliers.

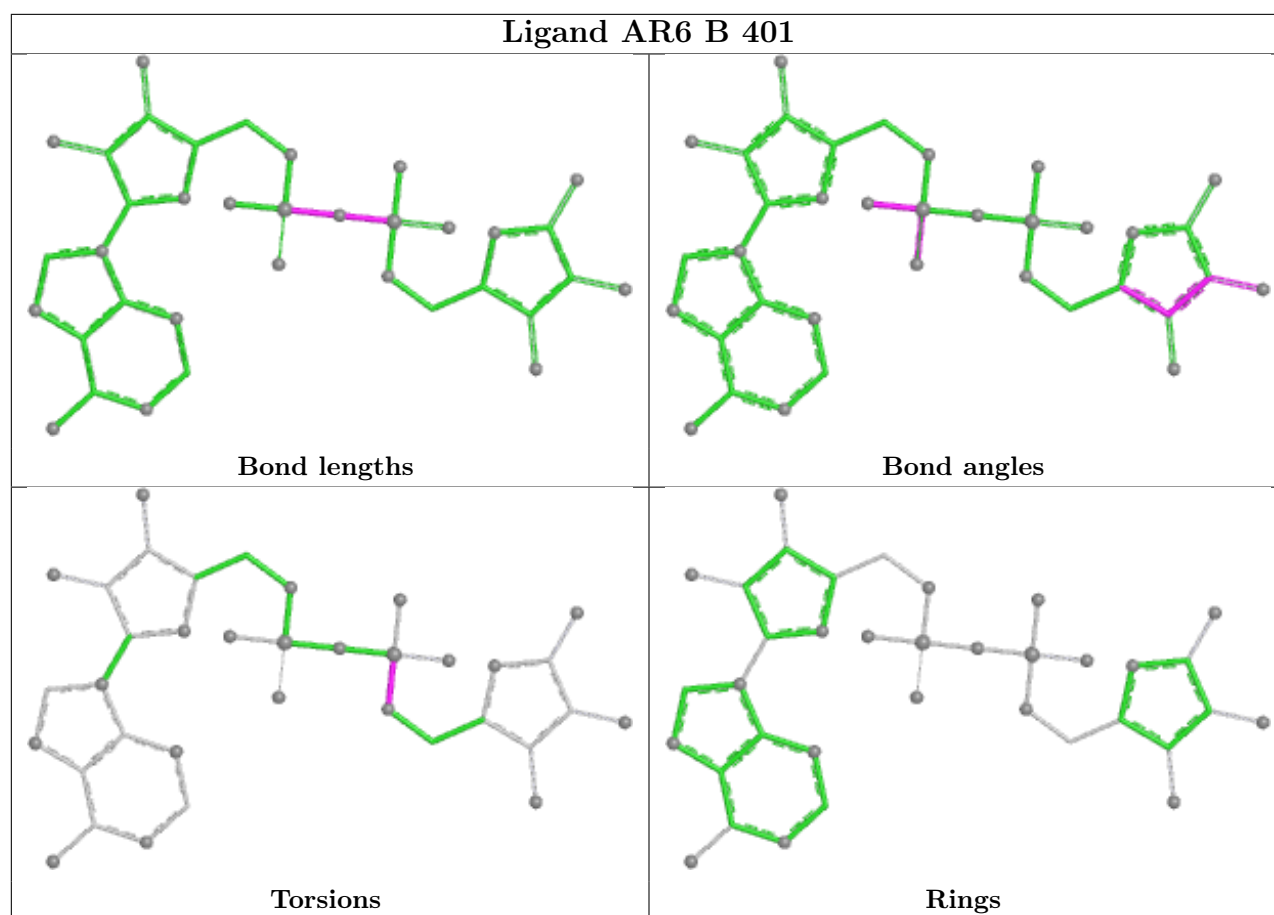
No monomer is involved in short contacts.

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	220:ARG	C	221:PRO	N	1.07

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

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

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

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

5.3 Carbohydrates [i](#)

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

5.4 Ligands [i](#)

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

5.5 Other polymers [i](#)

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