



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 01:29 AM EDT

PDB ID : 6MQ6
Title : Mapping the binding trajectory of a suicide inhibitor in human indoleamine 2,3-dioxygenase 1
Authors : Pham, K.N.; Yeh, S.R.
Deposited on : 2018-10-09
Resolution : 3.05 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 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 : 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) : 2.35.1

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 3.05 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 5 unique types of molecules in this entry. The entry contains 6114 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 Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	371	2943	1892	501	533	17	0	0	0
1	B	366	2915	1878	496	524	17	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	initiating methionine	UNP P14902
A	404	LYS	-	expression tag	UNP P14902
A	405	GLY	-	expression tag	UNP P14902
A	406	GLU	-	expression tag	UNP P14902
A	407	LEU	-	expression tag	UNP P14902
A	408	ASN	-	expression tag	UNP P14902
A	409	SER	-	expression tag	UNP P14902
A	410	LYS	-	expression tag	UNP P14902
A	411	LEU	-	expression tag	UNP P14902
A	412	GLU	-	expression tag	UNP P14902
A	413	GLY	-	expression tag	UNP P14902
A	414	LYS	-	expression tag	UNP P14902
A	415	PRO	-	expression tag	UNP P14902
A	416	ILE	-	expression tag	UNP P14902
A	417	PRO	-	expression tag	UNP P14902
A	418	ASN	-	expression tag	UNP P14902
A	419	PRO	-	expression tag	UNP P14902
A	420	LEU	-	expression tag	UNP P14902
A	421	LEU	-	expression tag	UNP P14902
A	422	GLY	-	expression tag	UNP P14902
A	423	LEU	-	expression tag	UNP P14902
A	424	ASP	-	expression tag	UNP P14902
A	425	SER	-	expression tag	UNP P14902
A	426	THR	-	expression tag	UNP P14902
A	427	ARG	-	expression tag	UNP P14902

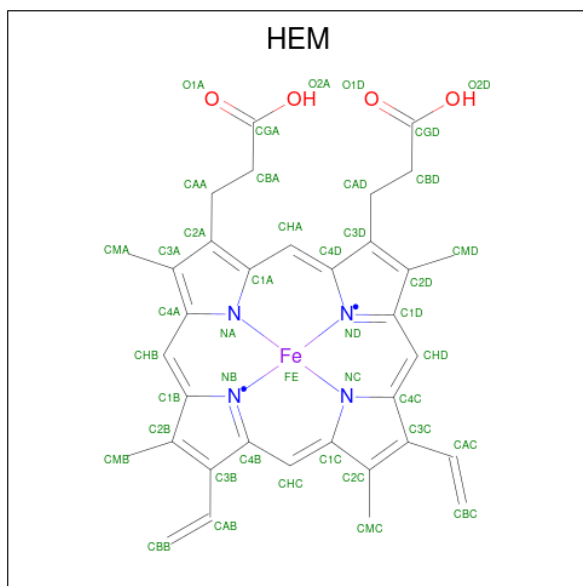
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Chain	Residue	Modelled	Actual	Comment	Reference
A	428	THR	-	expression tag	UNP P14902
A	429	GLY	-	expression tag	UNP P14902
A	430	HIS	-	expression tag	UNP P14902
A	431	HIS	-	expression tag	UNP P14902
A	432	HIS	-	expression tag	UNP P14902
A	433	HIS	-	expression tag	UNP P14902
A	434	HIS	-	expression tag	UNP P14902
A	435	HIS	-	expression tag	UNP P14902
B	11	MET	-	initiating methionine	UNP P14902
B	404	LYS	-	expression tag	UNP P14902
B	405	GLY	-	expression tag	UNP P14902
B	406	GLU	-	expression tag	UNP P14902
B	407	LEU	-	expression tag	UNP P14902
B	408	ASN	-	expression tag	UNP P14902
B	409	SER	-	expression tag	UNP P14902
B	410	LYS	-	expression tag	UNP P14902
B	411	LEU	-	expression tag	UNP P14902
B	412	GLU	-	expression tag	UNP P14902
B	413	GLY	-	expression tag	UNP P14902
B	414	LYS	-	expression tag	UNP P14902
B	415	PRO	-	expression tag	UNP P14902
B	416	ILE	-	expression tag	UNP P14902
B	417	PRO	-	expression tag	UNP P14902
B	418	ASN	-	expression tag	UNP P14902
B	419	PRO	-	expression tag	UNP P14902
B	420	LEU	-	expression tag	UNP P14902
B	421	LEU	-	expression tag	UNP P14902
B	422	GLY	-	expression tag	UNP P14902
B	423	LEU	-	expression tag	UNP P14902
B	424	ASP	-	expression tag	UNP P14902
B	425	SER	-	expression tag	UNP P14902
B	426	THR	-	expression tag	UNP P14902
B	427	ARG	-	expression tag	UNP P14902
B	428	THR	-	expression tag	UNP P14902
B	429	GLY	-	expression tag	UNP P14902
B	430	HIS	-	expression tag	UNP P14902
B	431	HIS	-	expression tag	UNP P14902
B	432	HIS	-	expression tag	UNP P14902
B	433	HIS	-	expression tag	UNP P14902
B	434	HIS	-	expression tag	UNP P14902
B	435	HIS	-	expression tag	UNP P14902

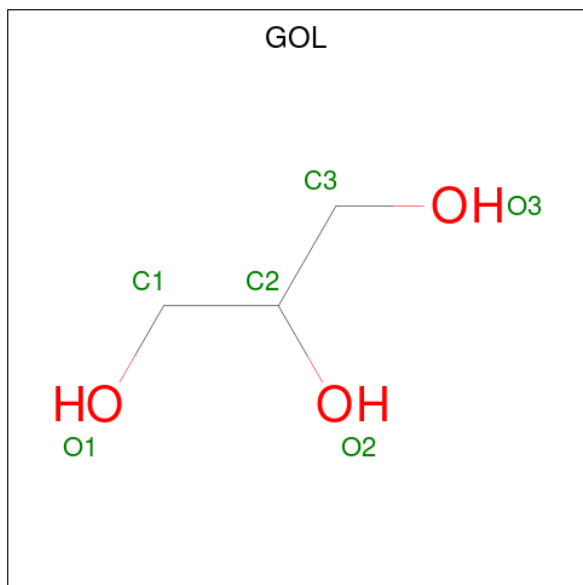
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



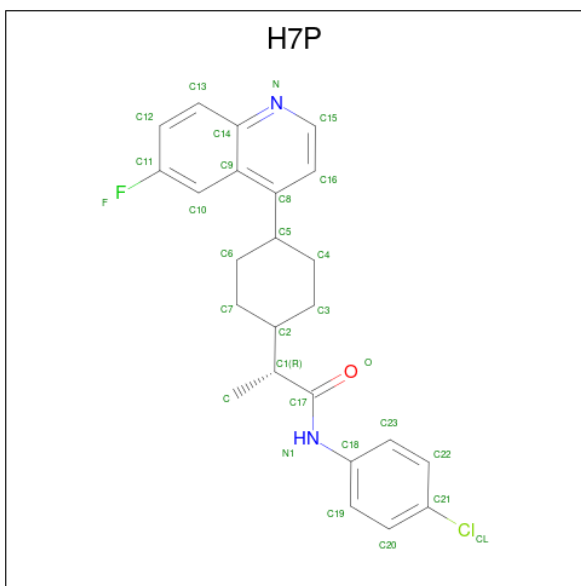
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
3	A	1	6	3	3	0	0

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

- Molecule 4 is (2R)-N-(4-chlorophenyl)-2-[cis-4-(6-fluoroquinolin-4-yl)cyclohexyl]propanamide (three-letter code: H7P) (formula: C₂₄H₂₄ClFN₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	B	1	Total	C	Cl	F	N	O	0	0
			29	24	1	1	2	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	78	Total	O	0	0
			78	78		

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	85.33Å 96.41Å 129.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 3.05	Depositor
% Data completeness (in resolution range)	99.6 (29.00-3.05)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.05Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.184 , 0.229	Depositor
Wilson B-factor (Å ²)	105.2	Xtrriage
Anisotropy	0.032	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	6114	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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 monosaccharides in this entry.

4.6 Ligand geometry [i](#)

8 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	GOL	A	503	-	5,5,5	0.26	0	5,5,5	0.26	0
3	GOL	B	504	-	5,5,5	0.28	0	5,5,5	0.21	0
2	HEM	A	501	5,1	41,50,50	1.31	4 (9%)	45,82,82	1.74	7 (15%)
3	GOL	A	502	-	5,5,5	0.29	0	5,5,5	0.21	0
3	GOL	B	505	-	5,5,5	0.30	0	5,5,5	0.20	0
3	GOL	B	502	-	5,5,5	0.26	0	5,5,5	0.23	0
3	GOL	B	503	-	5,5,5	0.30	0	5,5,5	0.14	0
4	H7P	B	501	-	32,32,32	1.45	5 (15%)	45,45,45	1.33	6 (13%)

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
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	B	504	-	-	2/4/4/4	-
2	HEM	A	501	5,1	-	4/12/54/54	-
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	B	505	-	-	2/4/4/4	-
3	GOL	B	502	-	-	2/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-
4	H7P	B	501	-	-	3/16/26/26	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	H7P	C9-C14	3.87	1.48	1.42
4	B	501	H7P	C8-C9	3.86	1.49	1.43
2	A	501	HEM	C1B-NB	-3.22	1.34	1.40
2	A	501	HEM	C4D-ND	-3.09	1.35	1.40
2	A	501	HEM	FE-NB	2.93	2.11	1.96
4	B	501	H7P	C18-N1	-2.82	1.35	1.41
4	B	501	H7P	C21-CL	2.45	1.79	1.74
4	B	501	H7P	C10-C11	2.35	1.40	1.36
2	A	501	HEM	CHB-C1B	2.16	1.40	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CHC-C4B-NB	5.05	129.91	124.43
4	B	501	H7P	C5-C8-C9	4.12	124.97	120.67
2	A	501	HEM	CHD-C1D-ND	4.02	128.79	124.43
2	A	501	HEM	C1B-NB-C4B	3.67	108.86	105.07
2	A	501	HEM	CHA-C4D-ND	3.35	128.52	124.38
4	B	501	H7P	C15-N-C14	3.23	121.94	116.93
2	A	501	HEM	CHB-C1B-NB	3.19	128.32	124.38
4	B	501	H7P	C9-C14-N	-2.74	119.91	122.83
2	A	501	HEM	CHD-C1D-C2D	-2.58	120.94	124.98
4	B	501	H7P	C16-C8-C5	-2.42	118.05	120.55
4	B	501	H7P	C3-C2-C7	2.33	113.55	109.44
2	A	501	HEM	CHA-C4D-C3D	-2.15	121.30	125.33
4	B	501	H7P	C18-N1-C17	-2.07	122.45	127.40

There are no chirality outliers.

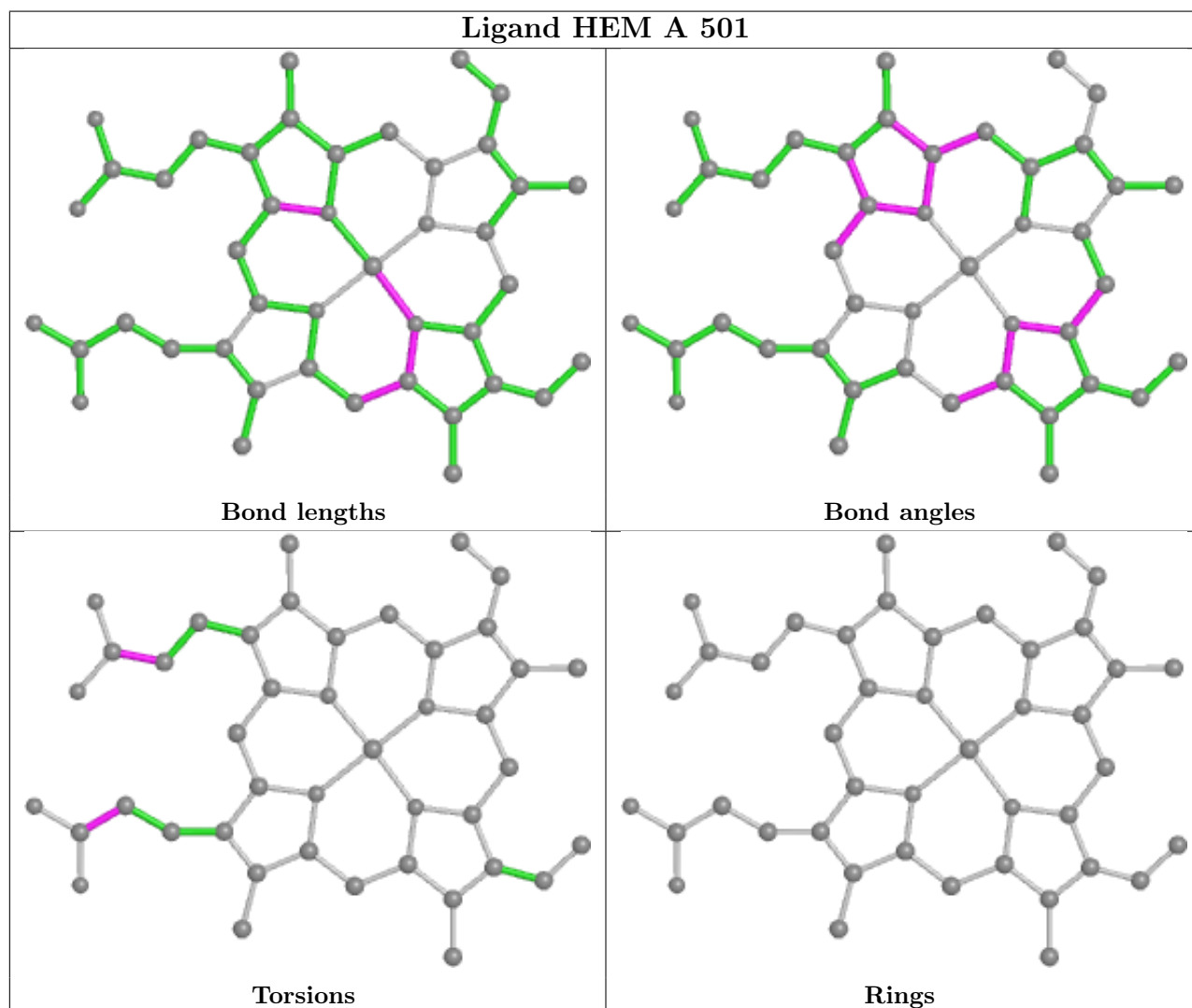
All (19) torsion outliers are listed below:

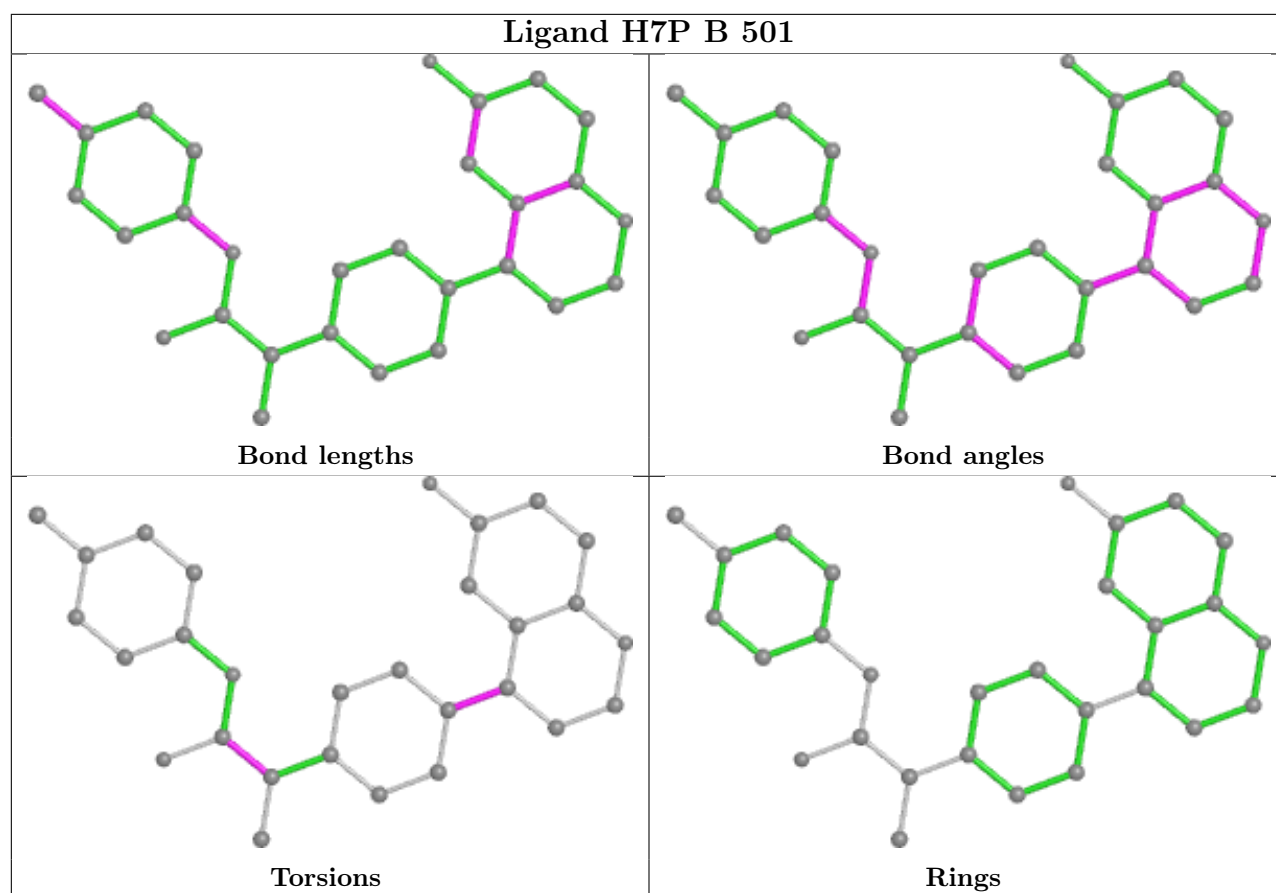
Mol	Chain	Res	Type	Atoms
3	B	502	GOL	O1-C1-C2-O2
3	B	502	GOL	O1-C1-C2-C3
3	B	503	GOL	O1-C1-C2-O2
3	B	503	GOL	O1-C1-C2-C3
3	B	504	GOL	O1-C1-C2-C3
3	B	505	GOL	O1-C1-C2-C3
4	B	501	H7P	C6-C5-C8-C9
4	B	501	H7P	C6-C5-C8-C16
3	A	503	GOL	O1-C1-C2-O2
3	B	504	GOL	O1-C1-C2-O2
3	A	502	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-C3
3	A	502	GOL	O2-C2-C3-O3
3	B	505	GOL	O1-C1-C2-O2
4	B	501	H7P	C-C1-C17-O
2	A	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAA-CBA-CGA-O2A

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](#)

There are no chain breaks in this entry.

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.