



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 02:49 PM EDT

PDB ID : 6NPN
Title : Crystal Structure of the Human vaccinia-related kinase bound to a N,N-dipropyl-dihydropteridine-3-hydroxyindazole inhibitor
Authors : Counago, R.M.; dos Reis, C.V.; Takarada, J.E.; Azevedo, A.; Guimaraes, C.; Mascarello, A.; Gama, F.; Ferreira, M.; Massirer, K.B.; Arruda, P.; Edwards, A.M.; Elkins, J.M.; Structural Genomics Consortium (SGC)
Deposited on : 2019-01-18
Resolution : 2.20 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)
Xtriage (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 2.20 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 10564 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 Serine/threonine-protein kinase VRK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	2472	1580	417	462	13	0	0	0
1	B	301	2345	1499	400	433	13	0	0	0
1	C	315	2469	1577	417	462	13	0	0	0
1	D	311	2437	1561	411	452	13	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

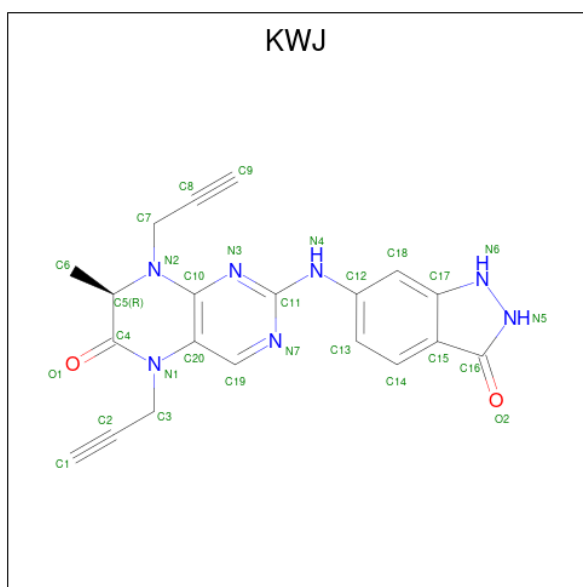
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q99986
A	2	MET	-	expression tag	UNP Q99986
A	34	ALA	LYS	engineered mutation	UNP Q99986
A	35	ALA	LYS	engineered mutation	UNP Q99986
A	36	ALA	GLU	engineered mutation	UNP Q99986
A	212	ALA	GLU	engineered mutation	UNP Q99986
A	214	ALA	LYS	engineered mutation	UNP Q99986
A	215	ALA	GLU	engineered mutation	UNP Q99986
A	292	ALA	GLU	engineered mutation	UNP Q99986
A	293	ALA	LYS	engineered mutation	UNP Q99986
A	295	ALA	LYS	engineered mutation	UNP Q99986
A	359	ALA	LYS	engineered mutation	UNP Q99986
A	360	ALA	LYS	engineered mutation	UNP Q99986
B	1	SER	-	expression tag	UNP Q99986
B	2	MET	-	expression tag	UNP Q99986
B	34	ALA	LYS	engineered mutation	UNP Q99986
B	35	ALA	LYS	engineered mutation	UNP Q99986
B	36	ALA	GLU	engineered mutation	UNP Q99986
B	212	ALA	GLU	engineered mutation	UNP Q99986
B	214	ALA	LYS	engineered mutation	UNP Q99986
B	215	ALA	GLU	engineered mutation	UNP Q99986

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Chain	Residue	Modelled	Actual	Comment	Reference
B	292	ALA	GLU	engineered mutation	UNP Q99986
B	293	ALA	LYS	engineered mutation	UNP Q99986
B	295	ALA	LYS	engineered mutation	UNP Q99986
B	359	ALA	LYS	engineered mutation	UNP Q99986
B	360	ALA	LYS	engineered mutation	UNP Q99986
C	1	SER	-	expression tag	UNP Q99986
C	2	MET	-	expression tag	UNP Q99986
C	34	ALA	LYS	engineered mutation	UNP Q99986
C	35	ALA	LYS	engineered mutation	UNP Q99986
C	36	ALA	GLU	engineered mutation	UNP Q99986
C	212	ALA	GLU	engineered mutation	UNP Q99986
C	214	ALA	LYS	engineered mutation	UNP Q99986
C	215	ALA	GLU	engineered mutation	UNP Q99986
C	292	ALA	GLU	engineered mutation	UNP Q99986
C	293	ALA	LYS	engineered mutation	UNP Q99986
C	295	ALA	LYS	engineered mutation	UNP Q99986
C	359	ALA	LYS	engineered mutation	UNP Q99986
C	360	ALA	LYS	engineered mutation	UNP Q99986
D	1	SER	-	expression tag	UNP Q99986
D	2	MET	-	expression tag	UNP Q99986
D	34	ALA	LYS	engineered mutation	UNP Q99986
D	35	ALA	LYS	engineered mutation	UNP Q99986
D	36	ALA	GLU	engineered mutation	UNP Q99986
D	212	ALA	GLU	engineered mutation	UNP Q99986
D	214	ALA	LYS	engineered mutation	UNP Q99986
D	215	ALA	GLU	engineered mutation	UNP Q99986
D	292	ALA	GLU	engineered mutation	UNP Q99986
D	293	ALA	LYS	engineered mutation	UNP Q99986
D	295	ALA	LYS	engineered mutation	UNP Q99986
D	359	ALA	LYS	engineered mutation	UNP Q99986
D	360	ALA	LYS	engineered mutation	UNP Q99986

- Molecule 2 is (7R)-7-methyl-2-[(3-oxo-2,3-dihydro-1H-indazol-6-yl)amino]-5,8-di(prop-2-yn-1-yl)-7,8-dihydropteridin-6(5H)-one (three-letter code: KWJ) (formula: C₂₀H₁₇N₇O₂).



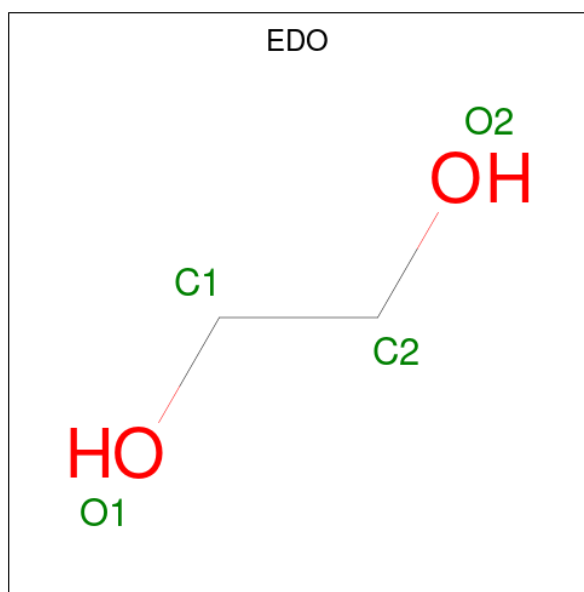
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
2	A	1	29	20	7	2	0	0
2	B	1	29	20	7	2	0	0
2	C	1	29	20	7	2	0	0
2	D	1	29	20	7	2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



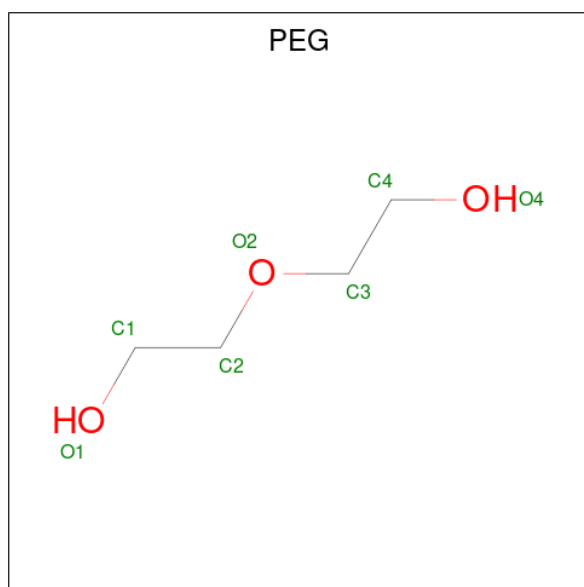
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	166	Total 166	O 166	0	0
6	B	123	Total 123	O 123	0	0
6	C	172	Total 172	O 172	0	0
6	D	157	Total 157	O 157	0	0

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

3 Data and refinement statistics i

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	92.53Å 96.32Å 191.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	99.8 (20.00-2.20)	Depositor
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.19Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.187 , 0.218	Depositor
Wilson B-factor (Å ²)	30.7	Xtrriage
Anisotropy	0.436	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.013 for k,h,-l	Xtrriage
Total number of atoms	10564	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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](#)

27 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	C	405	-	4,4,4	0.59	0	6,6,6	1.23	1 (16%)
3	SO4	C	402	-	4,4,4	0.13	0	6,6,6	1.02	0
3	SO4	D	402	-	4,4,4	0.36	0	6,6,6	0.37	0
4	EDO	B	406	-	3,3,3	0.70	0	2,2,2	0.32	0
2	KWJ	C	401	-	29,32,32	0.81	1 (3%)	34,46,46	0.98	2 (5%)
2	KWJ	D	401	-	29,32,32	0.81	1 (3%)	34,46,46	0.99	1 (2%)
3	SO4	B	402	-	4,4,4	0.47	0	6,6,6	0.30	0
5	PEG	B	405	-	6,6,6	0.95	0	5,5,5	0.94	0
2	KWJ	B	401	-	29,32,32	0.83	1 (3%)	34,46,46	1.04	3 (8%)
3	SO4	B	403	-	4,4,4	0.42	0	6,6,6	0.27	0
3	SO4	A	402	-	4,4,4	0.57	0	6,6,6	0.63	0
3	SO4	C	404	-	4,4,4	0.43	0	6,6,6	0.38	0
3	SO4	D	403	-	4,4,4	0.45	0	6,6,6	0.63	0
4	EDO	D	407	-	3,3,3	1.59	0	2,2,2	1.49	0
4	EDO	B	407	-	3,3,3	0.66	0	2,2,2	0.11	0
4	EDO	D	406	-	3,3,3	0.60	0	2,2,2	0.29	0
4	EDO	B	410	-	3,3,3	1.05	0	2,2,2	0.56	0
2	KWJ	A	401	-	29,32,32	0.81	1 (3%)	34,46,46	1.01	2 (5%)
3	SO4	D	405	-	4,4,4	0.73	0	6,6,6	0.82	0
4	EDO	C	406	-	3,3,3	0.68	0	2,2,2	0.02	0
3	SO4	D	404	-	4,4,4	0.38	0	6,6,6	0.46	0
3	SO4	C	403	-	4,4,4	0.55	0	6,6,6	0.53	0
4	EDO	B	408	-	3,3,3	0.49	0	2,2,2	0.30	0
3	SO4	B	404	-	4,4,4	0.50	0	6,6,6	0.32	0
4	EDO	B	409	-	3,3,3	0.13	0	2,2,2	1.17	0
4	EDO	C	407	-	3,3,3	0.70	0	2,2,2	0.18	0
4	EDO	A	403	-	3,3,3	0.55	0	2,2,2	0.20	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
4	EDO	B	410	-	-	0/1/1/1	-
2	KWJ	A	401	-	-	0/8/30/30	0/4/4/4
4	EDO	B	406	-	-	1/1/1/1	-
4	EDO	B	409	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KWJ	C	401	-	-	0/8/30/30	0/4/4/4
2	KWJ	D	401	-	-	0/8/30/30	0/4/4/4
4	EDO	C	407	-	-	1/1/1/1	-
4	EDO	B	407	-	-	0/1/1/1	-
4	EDO	D	407	-	-	1/1/1/1	-
4	EDO	C	406	-	-	1/1/1/1	-
5	PEG	B	405	-	-	4/4/4/4	-
2	KWJ	B	401	-	-	0/8/30/30	0/4/4/4
4	EDO	A	403	-	-	1/1/1/1	-
4	EDO	D	406	-	-	1/1/1/1	-
4	EDO	B	408	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	KWJ	C15-C16	-3.86	1.42	1.48
2	B	401	KWJ	C15-C16	-3.86	1.42	1.48
2	A	401	KWJ	C15-C16	-3.84	1.42	1.48
2	C	401	KWJ	C15-C16	-3.84	1.42	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	KWJ	C6-C5-N2	-2.50	109.43	112.34
2	C	401	KWJ	C6-C5-N2	-2.16	109.82	112.34
2	C	401	KWJ	C14-C15-C16	2.14	133.65	129.37
2	B	401	KWJ	C14-C15-C16	2.13	133.64	129.37
2	A	401	KWJ	C14-C15-C16	2.11	133.60	129.37
3	C	405	SO4	O4-S-O2	2.11	120.34	109.31
2	D	401	KWJ	C14-C15-C16	2.08	133.53	129.37
2	B	401	KWJ	C13-C12-C18	2.07	122.10	119.65
2	A	401	KWJ	C6-C5-N2	-2.02	109.98	112.34

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	406	EDO	O1-C1-C2-O2
4	D	407	EDO	O1-C1-C2-O2
4	A	403	EDO	O1-C1-C2-O2
4	B	408	EDO	O1-C1-C2-O2

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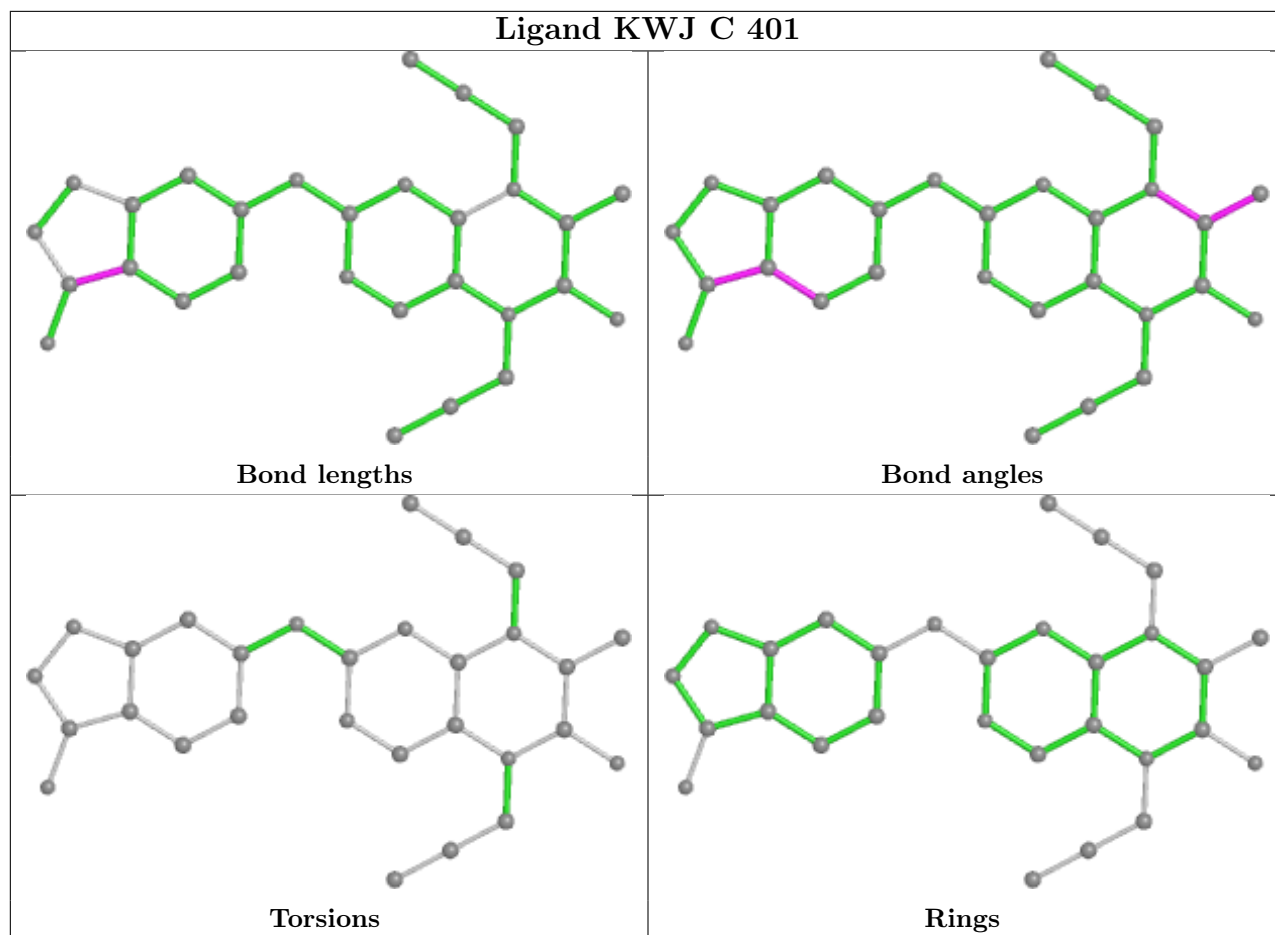
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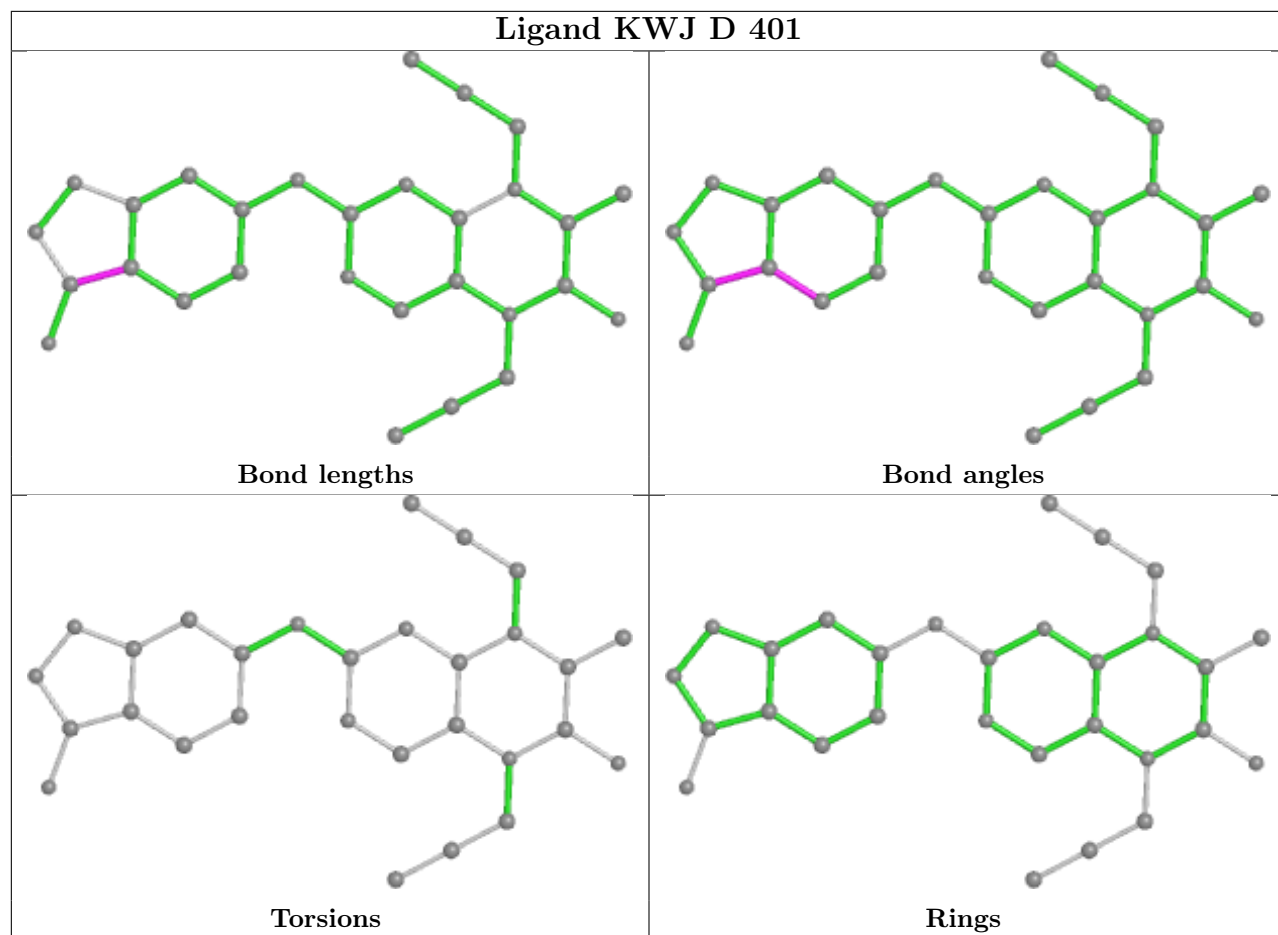
Mol	Chain	Res	Type	Atoms
5	B	405	PEG	O1-C1-C2-O2
5	B	405	PEG	O2-C3-C4-O4
4	B	406	EDO	O1-C1-C2-O2
5	B	405	PEG	C1-C2-O2-C3
4	D	406	EDO	O1-C1-C2-O2
5	B	405	PEG	C4-C3-O2-C2
4	C	407	EDO	O1-C1-C2-O2

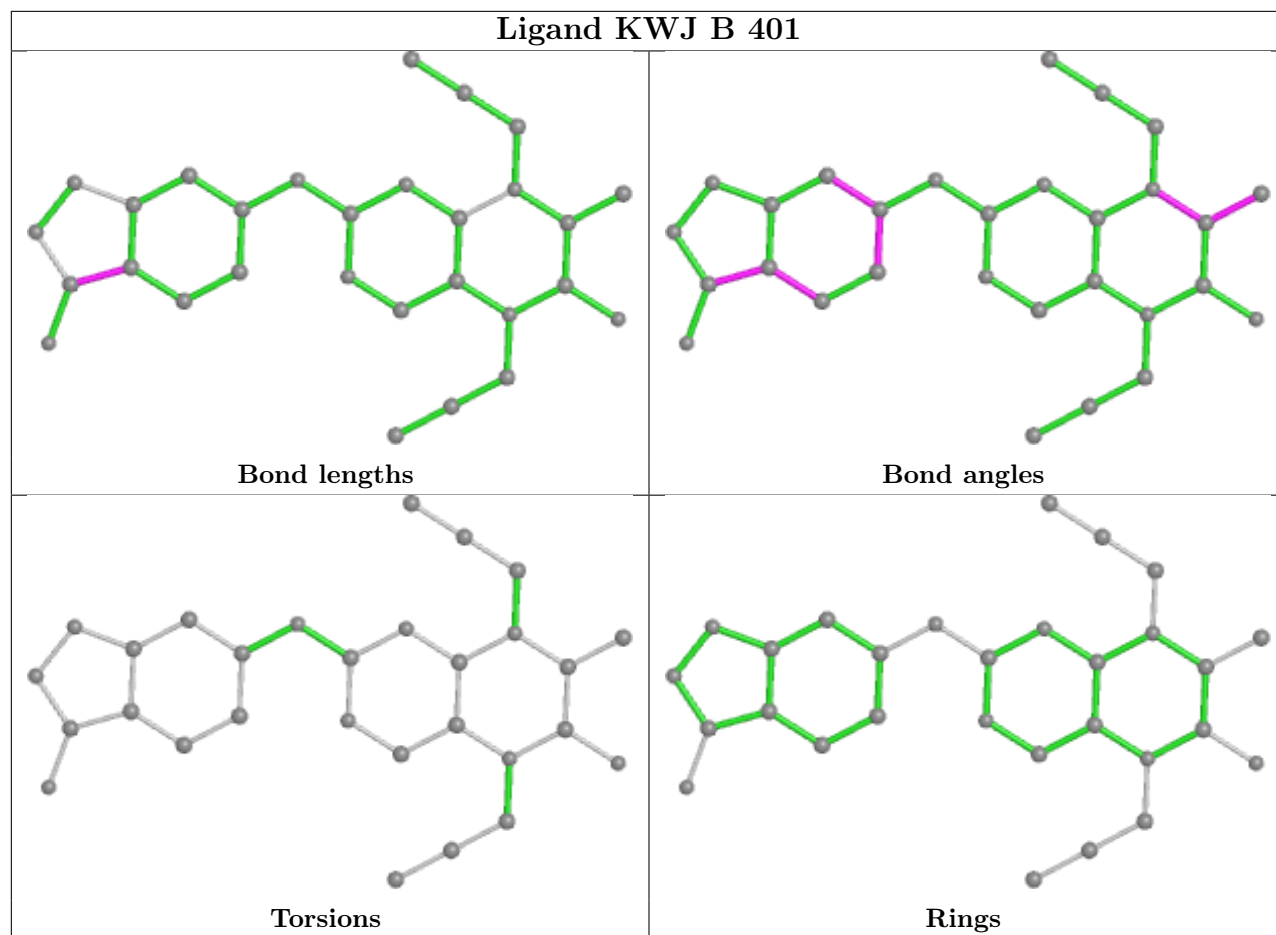
There are no ring outliers.

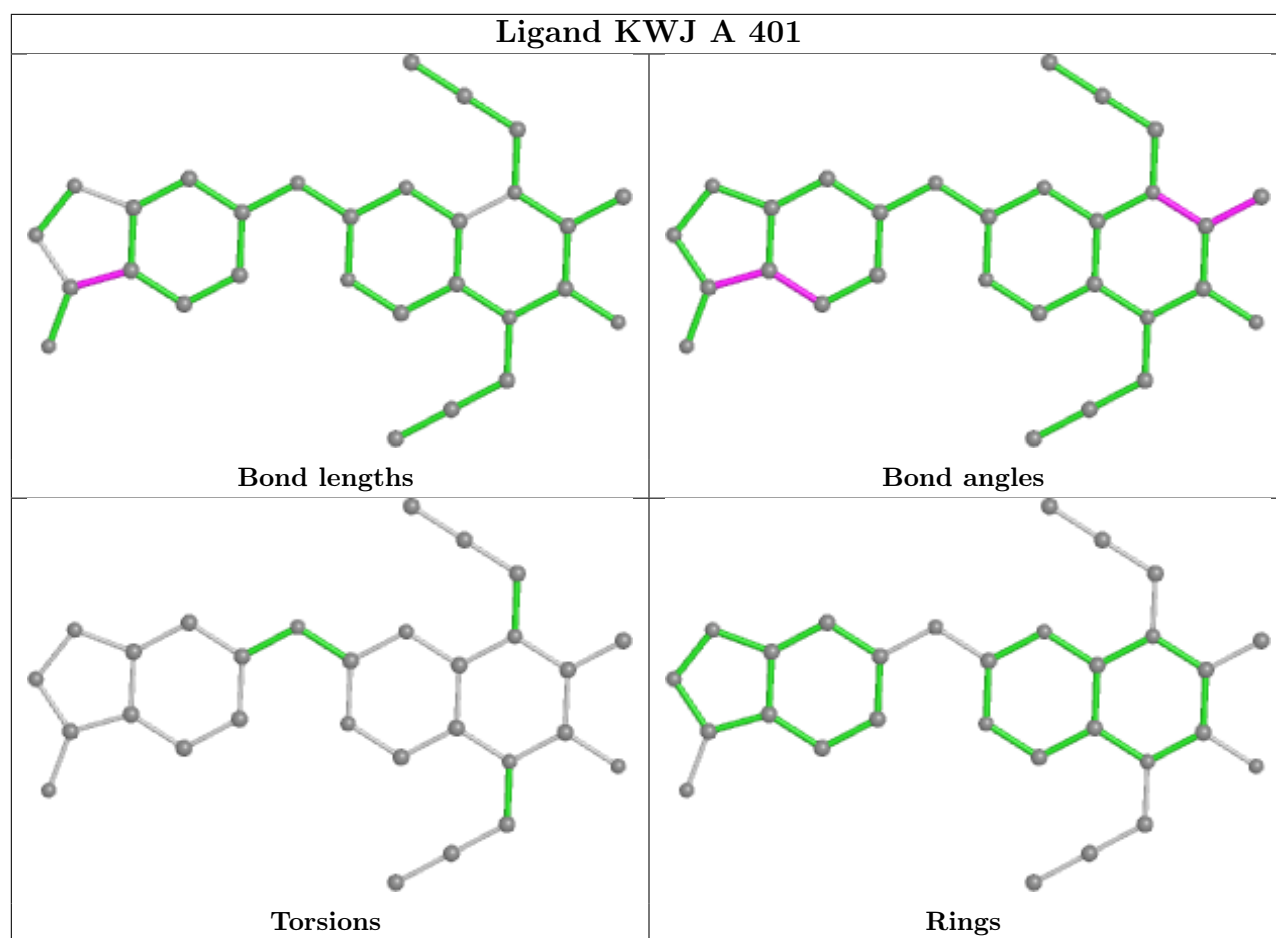
No monomer is involved in short contacts.

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 [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.