



# Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2020 – 09:21 pm BST

PDB ID : 5JNW  
Title : Crystal structure of bovine low molecular weight protein tyrosine phosphatase (LMPTP) mutant (W49Y N50E) complexed with vanadate and uncompetitive inhibitor  
Authors : Stanford, S.M.; Aleshin, A.E.; Liddington, R.C.; Bankston, L.; Cadwell, G.; Bottini, N.  
Deposited on : 2016-04-30  
Resolution : 1.86 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : **NOT EXECUTED**  
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) : 2.11

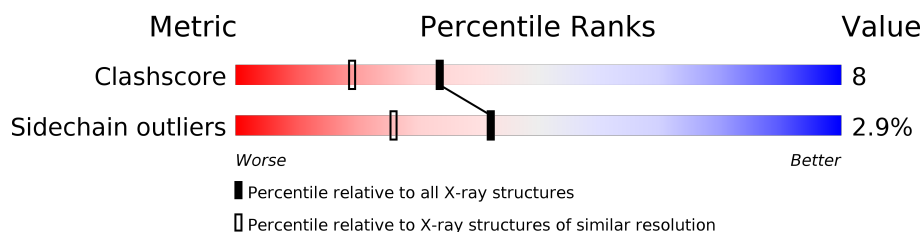
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 Å.


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2625 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	159	 73%      19%      . . .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1501 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.

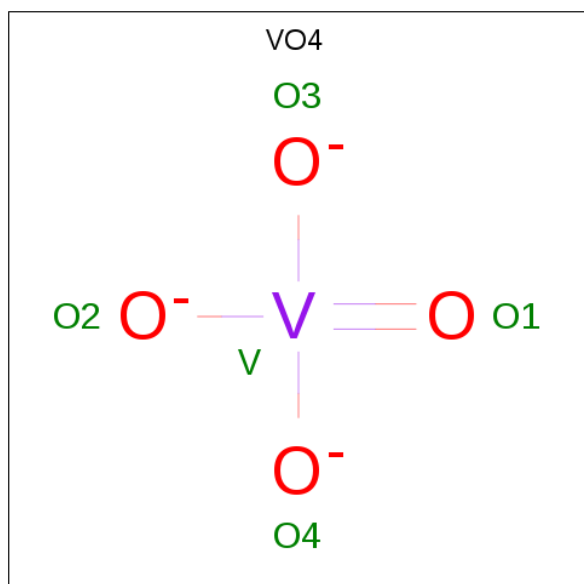
- Molecule 1 is a protein called Low molecular weight phosphotyrosine protein phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	6	0
			1288	801	227	251	9			

There are 4 discrepancies between the modelled and reference sequences:

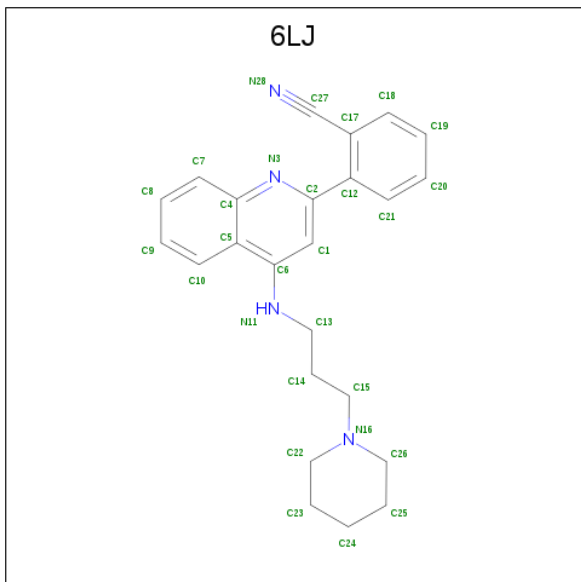
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P11064
A	0	SER	-	expression tag	UNP P11064
A	49	TYR	TRP	conflict	UNP P11064
A	50	GLU	ASN	conflict	UNP P11064

- Molecule 2 is VANADATE ION (three-letter code: VO4) (formula: O<sub>4</sub>V).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	V	0	0
			4	3	1		

- Molecule 3 is 2-(4-{[3-(piperidin-1-yl)propyl]amino}quinolin-2-yl)benzonitrile (three-letter code: 6LJ) (formula: C<sub>24</sub>H<sub>26</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	1
			56	48	8		

- Molecule 4 is water.

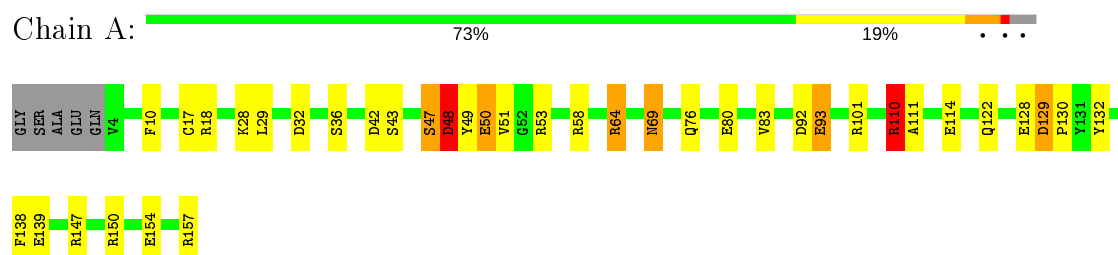
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	153	Total	O	0	0
			153	153		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: Low molecular weight phosphotyrosine protein phosphatase



## 4 Data and refinement statistics

EDS was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.35Å 125.49Å 45.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.70 – 1.86	Depositor
% Data completeness (in resolution range)	96.5 (36.70-1.86)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.166 , 0.209	Depositor
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.204	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.41% 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.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VO4, 6LJ

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  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.83	21/1310 (1.6%)	1.64	28/1770 (1.6%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93[A]	GLU	CD-OE2	9.38	1.35	1.25
1	A	93[B]	GLU	CD-OE2	9.38	1.35	1.25
1	A	64	ARG	CZ-NH1	8.45	1.44	1.33
1	A	147	ARG	CZ-NH1	8.36	1.44	1.33
1	A	154	GLU	CD-OE2	7.12	1.33	1.25
1	A	114	GLU	CD-OE2	-7.00	1.18	1.25
1	A	58	ARG	CD-NE	6.99	1.58	1.46
1	A	58	ARG	CZ-NH2	6.77	1.41	1.33
1	A	132[A]	TYR	CE1-CZ	6.40	1.46	1.38
1	A	132[B]	TYR	CE1-CZ	6.40	1.46	1.38
1	A	36	SER	CB-OG	-6.20	1.34	1.42
1	A	128	GLU	CD-OE1	5.94	1.32	1.25
1	A	111	ALA	N-CA	5.64	1.57	1.46
1	A	93[A]	GLU	CD-OE1	5.53	1.31	1.25
1	A	93[B]	GLU	CD-OE1	5.53	1.31	1.25
1	A	50[A]	GLU	CG-CD	5.47	1.60	1.51
1	A	50[B]	GLU	CG-CD	5.47	1.60	1.51
1	A	138	PHE	CG-CD1	5.33	1.46	1.38
1	A	80	GLU	CD-OE2	5.19	1.31	1.25
1	A	122	GLN	CG-CD	5.06	1.62	1.51
1	A	28	LYS	CD-CE	5.02	1.63	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ARG	NE-CZ-NH1	-13.43	113.59	120.30
1	A	128	GLU	OE1-CD-OE2	9.65	134.88	123.30
1	A	18	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	A	42	ASP	CB-CG-OD1	8.51	125.95	118.30
1	A	64	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	A	42	ASP	CB-CG-OD2	-8.17	110.95	118.30
1	A	64	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	A	147	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	A	58	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	157	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	29	LEU	CB-CG-CD2	7.16	123.16	111.00
1	A	132[A]	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	A	132[B]	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	A	69	ASN	CB-CA-C	-6.26	97.88	110.40
1	A	147	ARG	NH1-CZ-NH2	-6.24	112.54	119.40
1	A	47[A]	SER	C-N-CA	6.10	136.95	121.70
1	A	47[B]	SER	C-N-CA	6.10	136.95	121.70
1	A	139	GLU	OE1-CD-OE2	-6.08	116.01	123.30
1	A	101	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	18	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	48[A]	ASP	CB-CA-C	-5.66	99.09	110.40
1	A	48[B]	ASP	CB-CA-C	-5.66	99.09	110.40
1	A	147	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	32	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	150	ARG	CG-CD-NE	-5.48	100.30	111.80
1	A	129	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	92	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	110	ARG	NE-CZ-NH1	5.19	122.89	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1288	0	1249	21	0
2	A	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	56	0	0	8	0
4	A	153	0	0	1	0
All	All	1501	0	1249	22	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48[B]:ASP:OD2	4:A:301:HOH:O	1.61	1.14
1:A:48[B]:ASP:C	1:A:48[B]:ASP:OD1	1.93	0.98
1:A:49[A]:TYR:HA	3:A:202[A]:6LJ:C25	2.06	0.85
1:A:49[A]:TYR:HB3	3:A:202[A]:6LJ:C26	2.16	0.75
1:A:47[B]:SER:OG	1:A:49[B]:TYR:N	2.22	0.71
1:A:49[A]:TYR:CB	3:A:202[A]:6LJ:C26	2.79	0.61
1:A:49[A]:TYR:CA	3:A:202[A]:6LJ:C25	2.80	0.59
1:A:48[B]:ASP:OD1	1:A:49[B]:TYR:N	2.39	0.56
1:A:129:ASP:OD2	3:A:202[B]:6LJ:N3	2.39	0.56
1:A:83:VAL:O	1:A:110:ARG:NH2	2.41	0.54
1:A:48[B]:ASP:O	1:A:51:VAL:CG2	2.57	0.52
1:A:48[B]:ASP:HA	1:A:76:GLN:HB2	1.92	0.50
1:A:129:ASP:OD2	3:A:202[A]:6LJ:N3	2.44	0.50
1:A:50[A]:GLU:OE1	1:A:53:ARG:NH1	2.46	0.49
1:A:47[B]:SER:OG	1:A:48[B]:ASP:N	2.47	0.46
1:A:50[B]:GLU:HA	1:A:50[B]:GLU:OE1	2.16	0.46
3:A:202[A]:6LJ:C10	3:A:202[A]:6LJ:C13	2.93	0.45
1:A:49[A]:TYR:CG	3:A:202[A]:6LJ:C26	3.00	0.45
1:A:10:PHE:O	1:A:43:SER:HA	2.19	0.42
1:A:48[B]:ASP:O	1:A:51:VAL:HG23	2.19	0.42
1:A:17:CYS:HB2	2:A:201:VO4:O1	2.20	0.41
1:A:64:ARG:HH21	1:A:69:ASN:ND2	2.17	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	145/142 (102%)	139 (96%)	6 (4%)	30	13

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48[A]	ASP
1	A	48[B]	ASP
1	A	93[A]	GLU
1	A	93[B]	GLU
1	A	110	ARG
1	A	130	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	104	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

3 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	VO4	A	201	-	0,3,4	0.00	-	-		
3	6LJ	A	202[B]	-	31,31,31	2.43	7 (22%)	41,41,41	1.87	8 (19%)
3	6LJ	A	202[A]	-	31,31,31	2.63	8 (25%)	41,41,41	2.26	15 (36%)

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	6LJ	A	202[B]	-	-	0/13/21/21	0/4/4/4
3	6LJ	A	202[A]	-	-	6/13/21/21	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202[A]	6LJ	C15-N16	-10.92	1.22	1.47
3	A	202[B]	6LJ	C15-N16	-9.63	1.25	1.47
3	A	202[A]	6LJ	C17-C27	5.43	1.52	1.44
3	A	202[B]	6LJ	C17-C27	5.02	1.52	1.44
3	A	202[B]	6LJ	C6-N11	3.92	1.46	1.36
3	A	202[A]	6LJ	C6-N11	3.80	1.45	1.36
3	A	202[B]	6LJ	C4-N3	-3.16	1.32	1.37
3	A	202[A]	6LJ	C5-C4	-3.13	1.37	1.42
3	A	202[A]	6LJ	C4-N3	-2.78	1.33	1.37
3	A	202[A]	6LJ	C12-C2	2.70	1.55	1.48
3	A	202[B]	6LJ	C5-C4	-2.47	1.38	1.42
3	A	202[B]	6LJ	C12-C2	2.26	1.54	1.48
3	A	202[B]	6LJ	C25-C24	-2.20	1.42	1.51
3	A	202[A]	6LJ	C23-C24	-2.14	1.43	1.51
3	A	202[A]	6LJ	C25-C24	-2.02	1.43	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202[A]	6LJ	C6-C5-C4	6.81	122.37	118.06
3	A	202[B]	6LJ	C6-C5-C4	5.51	121.55	118.06
3	A	202[B]	6LJ	C5-C6-N11	4.71	125.16	119.66
3	A	202[A]	6LJ	C2-N3-C4	4.33	121.28	118.06
3	A	202[A]	6LJ	C18-C17-C27	-4.06	112.31	119.40
3	A	202[A]	6LJ	C10-C5-C6	-3.86	116.85	123.00
3	A	202[B]	6LJ	C18-C17-C27	-3.65	113.03	119.40
3	A	202[A]	6LJ	C25-C26-N16	3.64	117.17	111.33
3	A	202[B]	6LJ	C1-C2-C12	-3.61	117.41	122.25
3	A	202[A]	6LJ	C26-N16-C22	3.57	116.86	108.83
3	A	202[B]	6LJ	C1-C6-C5	-3.36	114.25	119.29
3	A	202[A]	6LJ	C1-C6-N11	3.26	126.76	121.59
3	A	202[B]	6LJ	C2-N3-C4	3.20	120.44	118.06
3	A	202[A]	6LJ	C1-C6-C5	-2.98	114.83	119.29
3	A	202[A]	6LJ	C12-C17-C27	2.95	127.47	121.75
3	A	202[B]	6LJ	C12-C17-C27	2.57	126.74	121.75
3	A	202[A]	6LJ	C14-C15-N16	-2.49	107.56	113.84
3	A	202[A]	6LJ	C5-C4-N3	-2.44	120.22	122.81
3	A	202[A]	6LJ	C15-N16-C22	2.35	117.25	111.23
3	A	202[A]	6LJ	C1-C2-C12	-2.26	119.22	122.25
3	A	202[A]	6LJ	C1-C2-N3	-2.20	120.22	122.23
3	A	202[A]	6LJ	C10-C5-C4	2.16	120.74	118.33
3	A	202[B]	6LJ	C25-C26-N16	2.04	114.59	111.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202[A]	6LJ	C5-C6-N11-C13
3	A	202[A]	6LJ	C1-C6-N11-C13
3	A	202[A]	6LJ	C13-C14-C15-N16
3	A	202[A]	6LJ	N11-C13-C14-C15
3	A	202[A]	6LJ	C14-C13-N11-C6
3	A	202[A]	6LJ	C14-C15-N16-C22

There are no ring outliers.

3 monomers are involved in 9 short contacts:

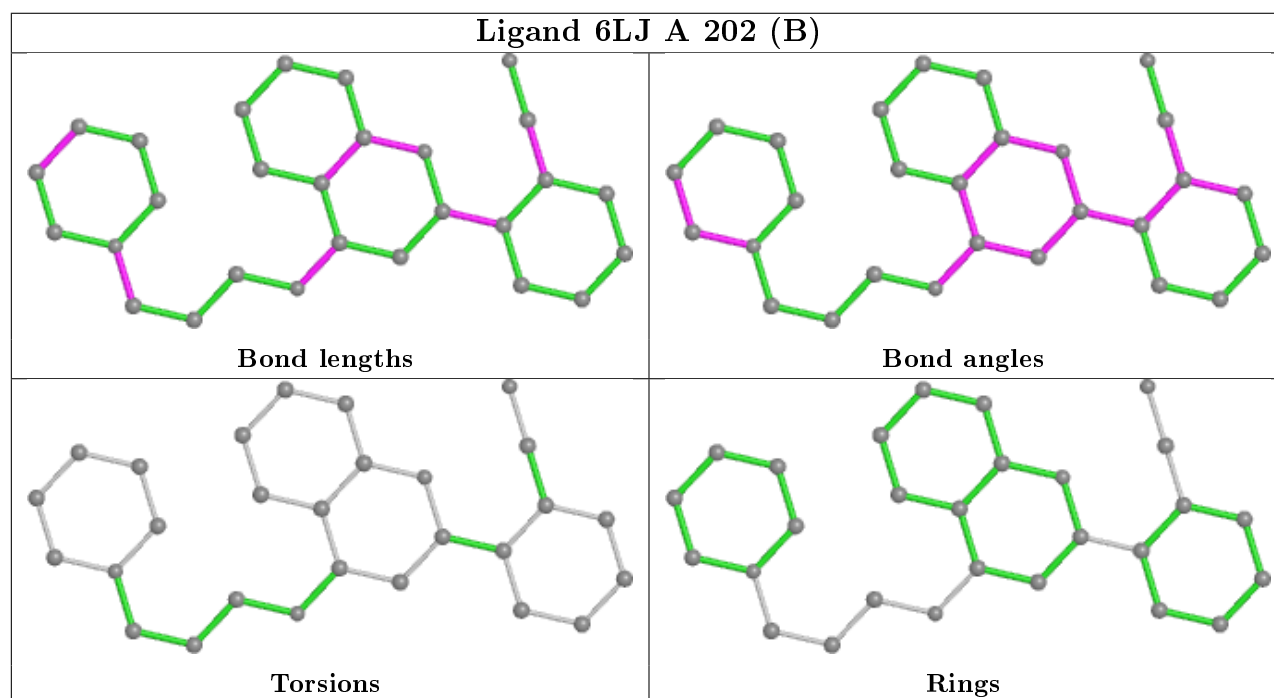
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	VO4	1	0

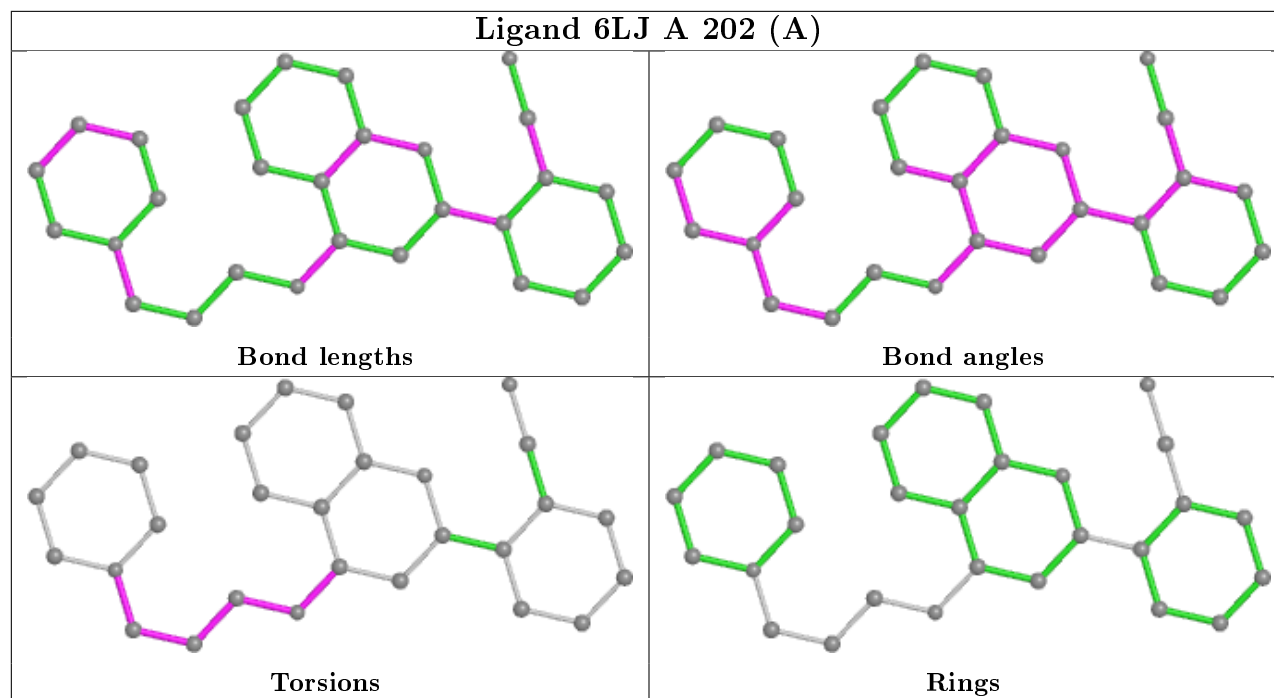
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202[B]	6LJ	1	0
3	A	202[A]	6LJ	7	0

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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.