



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 01:34 PM EDT

PDB ID : 1C86
Title : CRYSTAL STRUCTURE OF PROTEIN TYROSINE PHOSPHATASE 1B
(R47V,D48N) COMPLEXED WITH 2-(OXALYL-AMINO-4,7-DIHYDRO-5
H-THIENO[2,3-C]PYRAN-3-CARBOXYLIC ACID
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Deposited on : 2000-04-16
Resolution : 2.30 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 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) : **NOT EXECUTED**
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) : 2.23.2

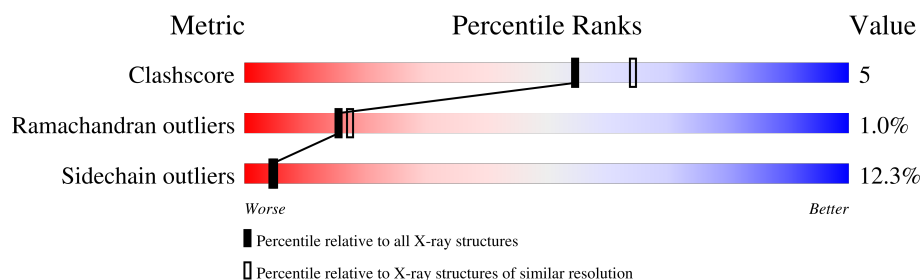
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	298	 70% 20% 7% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2560 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.

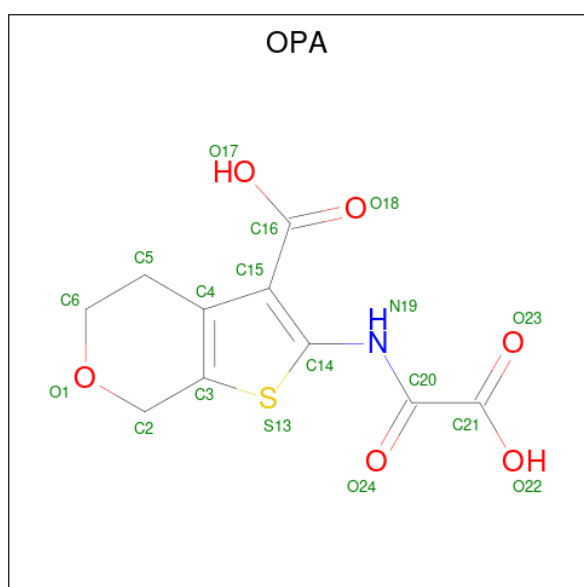
- Molecule 1 is a protein called PROTEIN (PROTEIN-TYROSINE PHOSPHATASE 1B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	296	2414	1529	415	454	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	VAL	ARG	engineered mutation	UNP P18031
A	48	ASN	ASP	engineered mutation	UNP P18031
A	151	THR	SER	conflict	UNP P18031
A	252	ASP	GLU	conflict	UNP P18031

- Molecule 2 is 2-(OXALYL-AMINO)-4,7-DIHYDRO-5H-THIENO[2,3-C]PYRAN-3-CARBOXYLIC ACID (three-letter code: OPA) (formula: C₁₀H₉NO₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			18	10	1	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: PROTEIN (PROTEIN-TYROSINE PHOSPHATASE 1B)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.27 Å 88.27 Å 104.50 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	98.5 (6.00-2.30)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.194 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2560	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OPA

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	1.12	16/2469 (0.6%)	1.67	37/3329 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	SER	CB-OG	7.37	1.51	1.42
1	A	21	GLN	CG-CD	6.53	1.66	1.51
1	A	285	SER	CB-OG	6.08	1.50	1.42
1	A	15	SER	CB-OG	5.95	1.50	1.42
1	A	201	SER	CB-OG	5.78	1.49	1.42
1	A	242	SER	CB-OG	5.73	1.49	1.42
1	A	93	GLY	CA-C	5.61	1.60	1.51
1	A	243	SER	CB-OG	5.25	1.49	1.42
1	A	50	SER	CB-OG	5.20	1.49	1.42
1	A	295	SER	CB-OG	5.13	1.49	1.42
1	A	13	SER	CB-OG	5.12	1.49	1.42
1	A	70	SER	CB-OG	5.12	1.49	1.42
1	A	190	SER	CB-OG	5.11	1.48	1.42
1	A	104	SER	CB-OG	5.09	1.48	1.42
1	A	286	SER	CB-OG	5.09	1.48	1.42
1	A	252	ASP	CB-CG	5.03	1.62	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	NE-CZ-NH1	14.75	127.68	120.30
1	A	254	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	A	205	SER	CB-CA-C	10.04	129.18	110.10
1	A	169	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	A	181	ASP	CB-CG-OD2	-9.49	109.76	118.30
1	A	160	LEU	CB-CG-CD2	8.87	126.07	111.00
1	A	238	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	A	25	HIS	CA-CB-CG	-8.77	98.69	113.60
1	A	199	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	A	81	TYR	CB-CG-CD1	-8.30	116.02	121.00
1	A	24	ARG	CD-NE-CZ	7.83	134.56	123.60
1	A	238	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	A	56	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	81	TYR	CB-CG-CD2	6.91	125.15	121.00
1	A	257	ARG	CD-NE-CZ	6.83	133.16	123.60
1	A	24	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	130	GLU	CB-CA-C	-6.75	96.91	110.40
1	A	47	VAL	CA-CB-CG2	6.66	120.88	110.90
1	A	45	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	A	297	GLU	N-CA-CB	6.52	122.34	110.60
1	A	271	TYR	CB-CG-CD1	-6.44	117.14	121.00
1	A	79	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	73	LYS	N-CA-CB	-6.25	99.35	110.60
1	A	156	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	43	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	268	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	132	GLU	CB-CA-C	-5.76	98.89	110.40
1	A	15	SER	N-CA-CB	-5.55	102.18	110.50
1	A	21	GLN	CB-CG-CD	5.47	125.81	111.60
1	A	168	THR	OG1-CB-CG2	5.35	122.31	110.00
1	A	43	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	254	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	245	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	140	LEU	CB-CG-CD1	5.14	119.75	111.00
1	A	162	ASN	CB-CA-C	5.09	120.57	110.40
1	A	49	VAL	CA-CB-CG1	5.08	118.52	110.90
1	A	45	ARG	NH1-CZ-NH2	-5.04	113.86	119.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	112	ARG	Sidechain
1	A	254	ARG	Sidechain

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	2414	0	2373	25	0
2	A	18	0	9	0	0
3	A	128	0	0	0	0
All	All	2560	0	2382	25	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 5.

All (25) 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:139:ASN:HD22	1:A:164:THR:HG22	1.40	0.87
1:A:139:ASN:ND2	1:A:164:THR:HG22	1.98	0.78
1:A:139:ASN:HD22	1:A:164:THR:CG2	2.14	0.57
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.69	0.55
1:A:17:ALA:O	1:A:21:GLN:HG3	2.06	0.55
1:A:7:PHE:CZ	1:A:272:LEU:HD13	2.44	0.52
1:A:45:ARG:H	1:A:85:GLN:HE22	1.56	0.51
1:A:205:SER:HB3	1:A:207:GLU:OE1	2.11	0.51
1:A:46:TYR:HB2	1:A:49:VAL:HG13	1.95	0.49
1:A:15:SER:O	1:A:19:ILE:HG12	2.13	0.48
1:A:12:LYS:HG2	1:A:13:SER:N	2.28	0.48
1:A:59:LEU:HB3	1:A:61:GLN:HG2	1.97	0.46
1:A:45:ARG:H	1:A:85:GLN:NE2	2.13	0.45
1:A:34:VAL:HG13	1:A:53:ASP:OD1	2.16	0.44
1:A:234:LEU:O	1:A:238:ARG:HG2	2.18	0.44
1:A:17:ALA:O	1:A:21:GLN:CG	2.66	0.43
1:A:128:LYS:HB3	1:A:128:LYS:HE2	1.67	0.43
1:A:167:GLU:HG2	1:A:168:THR:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:HG3	1:A:240:ASP:HB3	2.00	0.42
1:A:77:ALA:HB1	1:A:233:LEU:HD13	1.99	0.42
1:A:227:LEU:CD1	1:A:249:VAL:HG22	2.51	0.41
1:A:23:ILE:HG23	1:A:251:LEU:HD13	2.02	0.40
1:A:238:ARG:CD	1:A:243:SER:OG	2.70	0.40
1:A:100:TRP:HE3	1:A:160:LEU:HD13	1.86	0.40
1:A:153:TYR:HB2	1:A:175:HIS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran 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 backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	294/298 (99%)	284 (97%)	7 (2%)	3 (1%)	15 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	68	ASN
1	A	261	ILE

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	269/271 (99%)	236 (88%)	33 (12%)	4 5

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	12	LYS
1	A	15	SER
1	A	34	VAL
1	A	49	VAL
1	A	59	LEU
1	A	71	LEU
1	A	72	ILE
1	A	88	LEU
1	A	105	ARG
1	A	128	LYS
1	A	130	GLU
1	A	131	LYS
1	A	132	GLU
1	A	140	LEU
1	A	158	LEU
1	A	160	LEU
1	A	163	LEU
1	A	164	THR
1	A	168	THR
1	A	172	LEU
1	A	175	HIS
1	A	197	LYS
1	A	233	LEU
1	A	234	LEU
1	A	237	LYS
1	A	244	VAL
1	A	249	VAL
1	A	251	LEU
1	A	252	ASP
1	A	270	SER
1	A	272	LEU
1	A	294	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	111	ASN
1	A	139	ASN
1	A	162	ASN
1	A	166	GLN
1	A	175	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	OPA	A	301	-	12,19,19	4.44	4 (33%)	8,27,27	2.76	2 (25%)

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
2	OPA	A	301	-	-	0/2/19/19	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	OPA	O24-C20	10.93	1.45	1.23
2	A	301	OPA	C15-C16	-9.28	1.38	1.47
2	A	301	OPA	C5-C4	-4.07	1.45	1.51
2	A	301	OPA	C2-C3	-3.21	1.45	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	OPA	C21-C20-N19	6.16	120.34	113.74
2	A	301	OPA	C6-C5-C4	-3.53	105.58	110.82

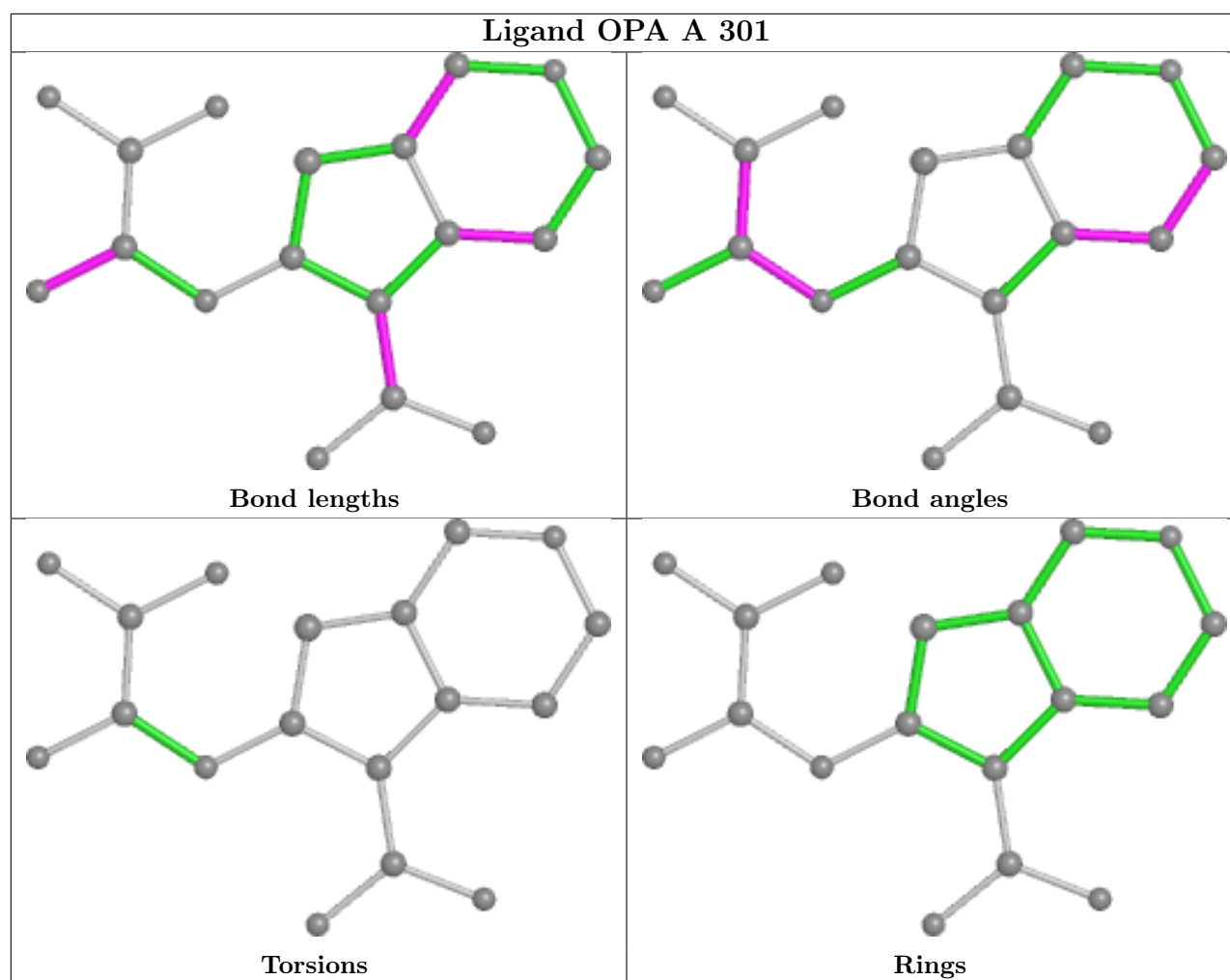
There are no chirality outliers.

There are no torsion outliers.

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.



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.