



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:06 PM UTC

PDB ID : 1C87 / pdb_00001c87
Title : CRYSTAL STRUCTURE OF PROTEIN TYROSINE PHOSPHATASE 1B
COMPLEXED WITH 2-(OXALYL-AMINO-4,7-DIHYDRO-5H-THIENO[2,3
-C]PYRAN-3-CARBOXYLIC ACID
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Deposited on : 2000-04-16
Resolution : 2.10 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

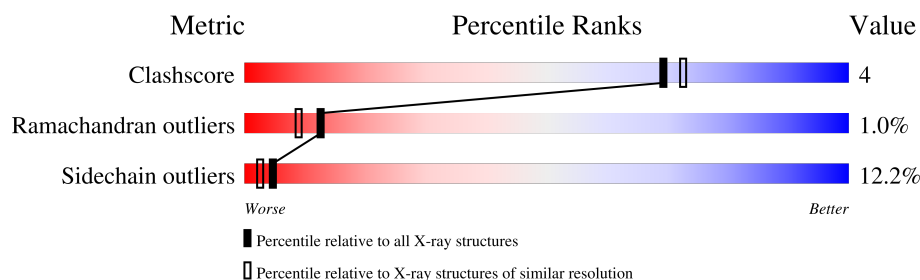
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	 67% 27% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2628 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.

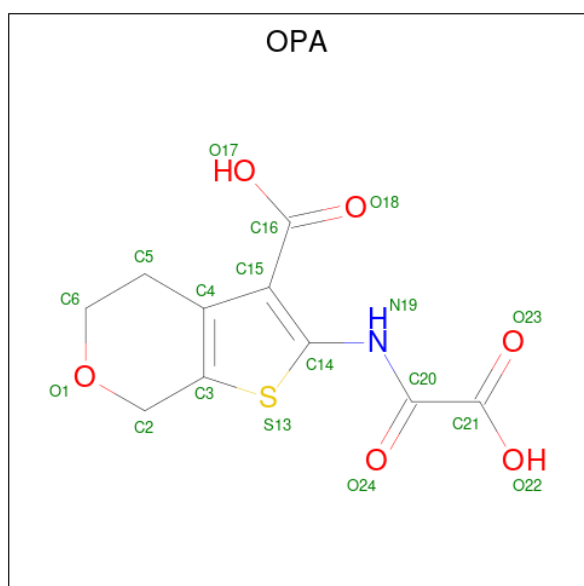
- Molecule 1 is a protein called PROTEIN (PROTEIN-TYROSINE PHOSPHATASE 1B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2427	1535	418	458	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 (CCD ID: 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	183	Total 183	O 183	0	0

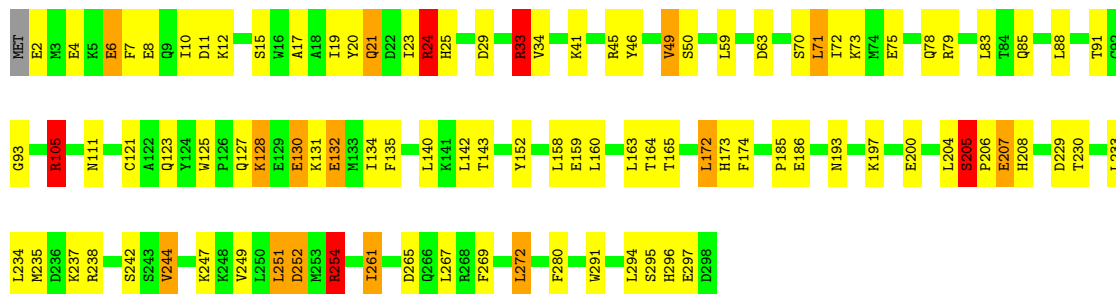
3 Residue-property plots

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)

Chain A: 



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	87.90 Å 87.90 Å 103.09 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.10	Depositor
% Data completeness (in resolution range)	98.4 (6.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.194 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2628	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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	1.59	27/2482 (1.1%)	1.91	45/3345 (1.3%)

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	9

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	GLU	CA-C	9.00	1.64	1.52
1	A	50	SER	C-O	-7.94	1.13	1.24
1	A	24	ARG	NE-CZ	6.57	1.40	1.33
1	A	173	HIS	CG-ND1	-6.53	1.31	1.38
1	A	152	TYR	CA-C	6.30	1.60	1.52
1	A	127	GLN	CA-C	6.22	1.61	1.52
1	A	252	ASP	CA-CB	6.02	1.62	1.53
1	A	185	PRO	CA-C	5.97	1.59	1.52
1	A	296	HIS	CG-CD2	5.86	1.42	1.35
1	A	143	THR	CA-C	-5.59	1.45	1.52
1	A	121	CYS	CA-C	5.41	1.59	1.52
1	A	125	TRP	C-N	5.35	1.40	1.33
1	A	130	GLU	N-CA	5.32	1.53	1.46
1	A	50	SER	C-N	5.32	1.40	1.33
1	A	242	SER	CB-OG	5.30	1.52	1.42
1	A	93	GLY	CA-C	5.30	1.58	1.52
1	A	193	ASN	CA-C	5.28	1.59	1.52
1	A	125	TRP	CA-C	5.26	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	THR	CA-C	-5.26	1.46	1.52
1	A	267	LEU	N-CA	5.21	1.52	1.46
1	A	235	MET	CA-C	5.16	1.59	1.52
1	A	21	GLN	CG-CD	5.16	1.65	1.52
1	A	41	LYS	CA-C	5.14	1.59	1.52
1	A	25	HIS	CG-CD2	5.09	1.41	1.35
1	A	75	GLU	CA-C	5.06	1.59	1.52
1	A	280	PHE	CA-C	5.02	1.59	1.52
1	A	265	ASP	CA-C	5.01	1.59	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	HIS	CA-CB-CG	-15.37	98.43	113.80
1	A	21	GLN	CB-CG-CD	8.26	126.64	112.60
1	A	244	VAL	N-CA-CB	8.13	120.27	111.00
1	A	130	GLU	CB-CG-CD	7.58	125.48	112.60
1	A	297	GLU	N-CA-CB	7.18	120.79	110.16
1	A	78	GLN	OE1-CD-NE2	7.17	129.77	122.60
1	A	49	VAL	CA-C-O	7.03	126.48	120.22
1	A	254	ARG	NE-CZ-NH1	6.79	128.29	121.50
1	A	29	ASP	N-CA-CB	-6.61	100.59	110.90
1	A	252	ASP	N-CA-CB	6.56	119.77	110.12
1	A	8	GLU	CB-CA-C	6.50	122.59	110.70
1	A	132	GLU	CB-CA-C	-6.49	96.22	109.65
1	A	200	GLU	N-CA-CB	-6.34	100.80	110.12
1	A	208	HIS	CA-CB-CG	-6.30	107.50	113.80
1	A	265	ASP	CA-CB-CG	-6.26	106.34	112.60
1	A	193	ASN	CB-CA-C	6.07	120.57	110.92
1	A	123	GLN	OE1-CD-NE2	-6.01	116.59	122.60
1	A	200	GLU	CA-C-O	5.91	126.82	120.55
1	A	125	TRP	CB-CA-C	5.90	118.01	108.87
1	A	254	ARG	NE-CZ-NH2	-5.83	113.95	119.20
1	A	25	HIS	N-CA-C	5.81	118.56	111.82
1	A	269	PHE	CA-CB-CG	-5.71	108.09	113.80
1	A	10	ILE	N-CA-CB	5.67	117.82	110.57
1	A	143	THR	OG1-CB-CG2	-5.64	98.02	109.30
1	A	111	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	6	GLU	CB-CG-CD	5.61	122.14	112.60
1	A	49	VAL	N-CA-CB	5.59	119.60	112.34
1	A	70	SER	CB-CA-C	-5.54	97.81	109.38
1	A	207	GLU	N-CA-C	5.54	119.14	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	TYR	CB-CA-C	5.52	119.50	110.17
1	A	193	ASN	CB-CG-ND2	5.50	124.65	116.40
1	A	164	THR	CA-C-N	-5.49	113.99	122.49
1	A	164	THR	C-N-CA	-5.49	113.99	122.49
1	A	29	ASP	CB-CA-C	5.42	118.54	110.62
1	A	33	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	A	267	LEU	CA-C-O	5.32	126.40	120.82
1	A	244	VAL	CA-CB-CG1	5.30	119.41	110.40
1	A	242	SER	CA-CB-OG	5.26	121.62	111.10
1	A	33	ARG	NH1-CZ-NH2	5.22	126.09	119.30
1	A	165	THR	N-CA-CB	-5.22	102.73	110.61
1	A	29	ASP	CA-CB-CG	-5.21	107.39	112.60
1	A	91	THR	CA-CB-OG1	5.17	117.35	109.60
1	A	105	ARG	N-CA-CB	-5.12	103.01	110.53
1	A	229	ASP	CA-CB-CG	-5.11	107.49	112.60
1	A	135	PHE	CA-CB-CG	5.05	118.85	113.80

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	204	LEU	Peptide
1	A	205	SER	Peptide
1	A	238	ARG	Sidechain
1	A	24	ARG	Sidechain
1	A	254	ARG	Sidechain
1	A	33	ARG	Sidechain
1	A	46	TYR	Sidechain
1	A	79	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	2427	0	2381	17	0
2	A	18	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	183	0	0	0	0
All	All	2628	0	2388	17	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 4.

All (17) 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:45:ARG:H	1:A:85:GLN:HE22	1.50	0.57
1:A:17:ALA:O	1:A:21:GLN:HG3	2.06	0.56
1:A:2:GLU:HG3	1:A:4:GLU:H	1.74	0.52
1:A:105:ARG:HH11	1:A:105:ARG:HG2	1.75	0.52
1:A:45:ARG:H	1:A:85:GLN:NE2	2.07	0.52
1:A:6:GLU:CD	1:A:247:LYS:HZ2	2.19	0.50
1:A:7:PHE:CZ	1:A:272:LEU:HD13	2.48	0.48
1:A:205:SER:O	1:A:207:GLU:N	2.48	0.46
1:A:71:LEU:HD13	1:A:73:LYS:HB2	1.98	0.45
1:A:291:TRP:O	1:A:295:SER:HB3	2.16	0.45
1:A:172:LEU:HB3	1:A:174:PHE:CE1	2.51	0.45
1:A:23:ILE:HG23	1:A:251:LEU:HD13	2.01	0.43
1:A:15:SER:O	1:A:19:ILE:HG12	2.19	0.43
1:A:128:LYS:HB3	1:A:128:LYS:HE2	1.75	0.42
1:A:142:LEU:HA	1:A:159:GLU:O	2.21	0.41
1:A:83:LEU:HD12	1:A:83:LEU:N	2.36	0.41
1:A:20:TYR:CE2	1:A:24:ARG:HD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	295/298 (99%)	280 (95%)	12 (4%)	3 (1%)	12 9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	261	ILE
1	A	206	PRO

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	270/271 (100%)	237 (88%)	33 (12%)	5 2

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	33	ARG
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	128	LYS
1	A	130	GLU
1	A	131	LYS
1	A	132	GLU
1	A	134	ILE
1	A	140	LEU
1	A	158	LEU
1	A	160	LEU
1	A	163	LEU

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Mol	Chain	Res	Type
1	A	172	LEU
1	A	186	GLU
1	A	197	LYS
1	A	205	SER
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	254	ARG
1	A	261	ILE
1	A	272	LEU
1	A	294	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	78	GLN
1	A	85	GLN
1	A	111	ASN
1	A	123	GLN
1	A	175	HIS
1	A	262	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	-	19,19,19	2.24	6 (31%)	24,27,27	3.10	14 (58%)

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	-	-	3/11/19/19	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	OPA	O23-C21	5.77	1.36	1.22
2	A	301	OPA	O22-C21	-3.89	1.20	1.30
2	A	301	OPA	C20-C21	3.19	1.57	1.54
2	A	301	OPA	C14-N19	3.06	1.42	1.38
2	A	301	OPA	C15-C14	-2.89	1.34	1.39
2	A	301	OPA	C14-S13	-2.64	1.69	1.73

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	OPA	C14-C15-C4	-7.82	107.72	111.75
2	A	301	OPA	C15-C14-N19	-5.41	119.22	124.61
2	A	301	OPA	C6-C5-C4	-4.74	102.98	108.87
2	A	301	OPA	C3-S13-C14	-4.28	88.95	91.14
2	A	301	OPA	C20-N19-C14	3.85	128.29	125.26
2	A	301	OPA	C15-C14-S13	3.82	117.64	112.62
2	A	301	OPA	O1-C2-C3	-3.69	105.73	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	OPA	C5-C4-C15	-3.24	122.00	127.16
2	A	301	OPA	C5-C4-C3	3.07	124.61	121.39
2	A	301	OPA	O17-C16-O18	-2.60	117.70	123.90
2	A	301	OPA	O17-C16-C15	2.47	122.90	116.58
2	A	301	OPA	C16-C15-C14	2.22	123.38	120.09
2	A	301	OPA	C2-C3-C4	2.17	126.18	122.44
2	A	301	OPA	O24-C20-N19	2.12	126.68	122.88

There are no chirality outliers.

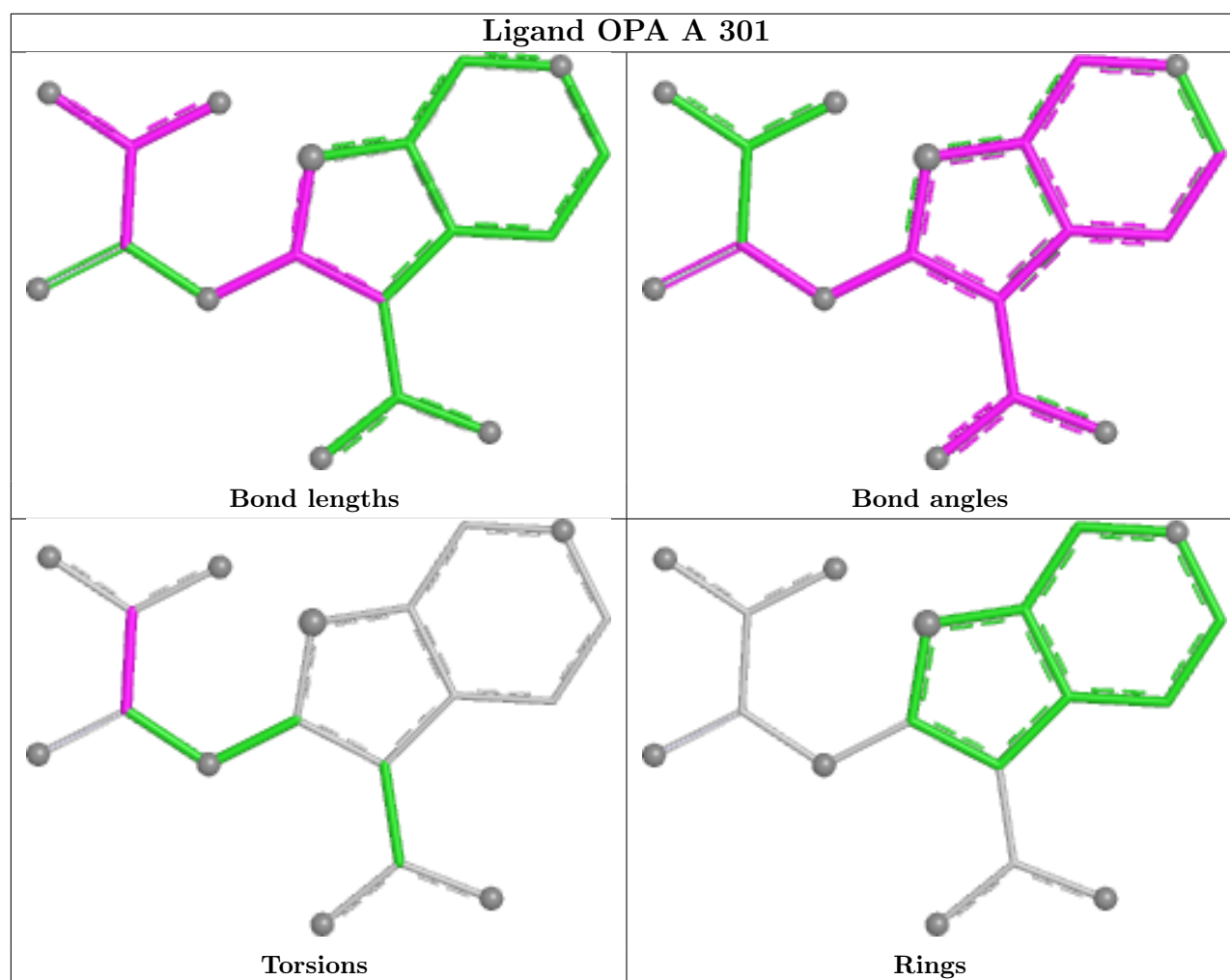
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	OPA	N19-C20-C21-O23
2	A	301	OPA	O24-C20-C21-O22
2	A	301	OPA	O24-C20-C21-O23

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.