



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:08 AM UTC

PDB ID : 1ECV / pdb_00001ecv
Title : CRYSTAL STRUCTURE OF PROTEIN TYROSINE PHOSPHATASE 1B
COMPLEXED WITH 5-iodo-2-(oxalyl-amino)-benzoic acid
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Deposited on : 2000-01-26
Resolution : 1.95 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

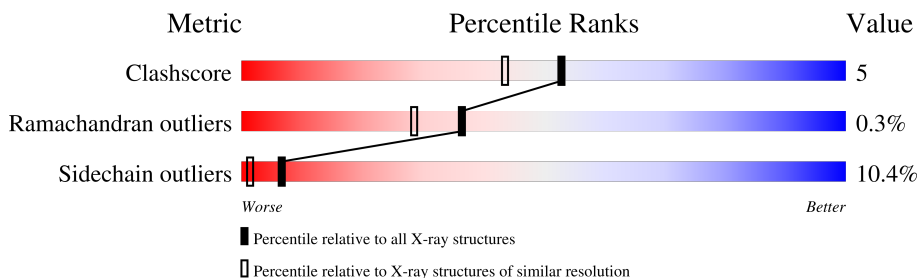
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)

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	 64% 25% 10% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2724 atoms, of which 28 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.

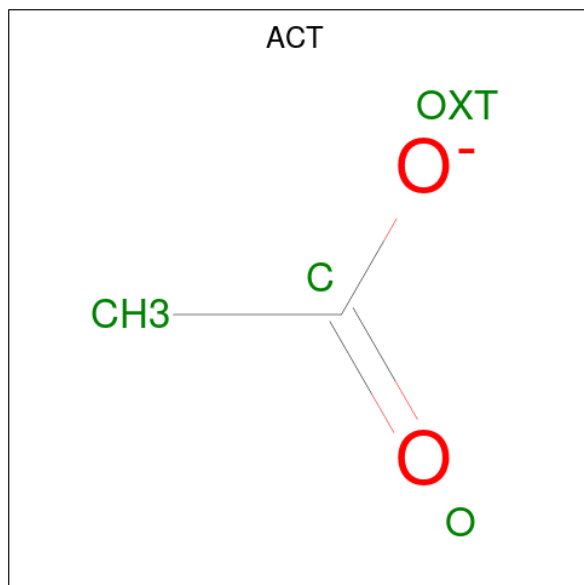
- Molecule 1 is a protein called PROTEIN-TYROSINE PHOSPHATASE 1B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	297	2455	1535	28	418	458	16	0	0	0

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 ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



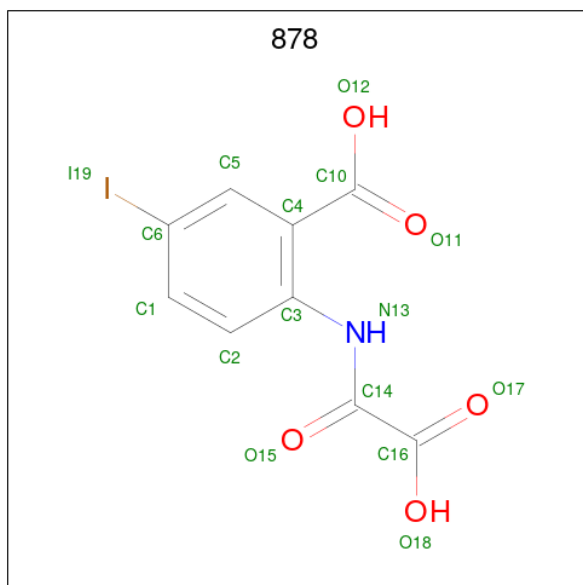
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 3 is 5-iodo-2-(oxalyl-amino)-benzoic acid (CCD ID: 878) (formula: $C_9H_6INO_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	I	N	O	0	0
			16	9	1	1	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	241	Total	O	0	0
			241	241		

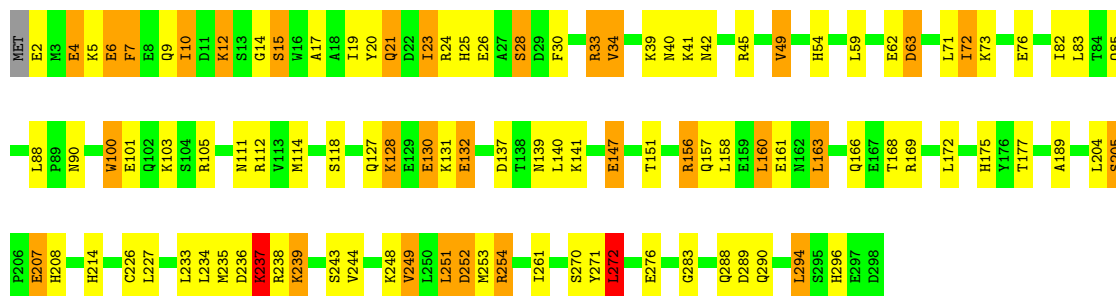
3 Residue-property plots

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-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	87.87Å 87.87Å 103.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 1.95	Depositor
% Data completeness (in resolution range)	99.5 (6.00-1.95)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.194 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2724	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: ACT, 878

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	1.36	12/2482 (0.5%)	2.04	89/3345 (2.7%)

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	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	HIS	CE1-NE2	7.53	1.40	1.32
1	A	25	HIS	ND1-CE1	7.18	1.39	1.32
1	A	128	LYS	CA-C	-6.95	1.44	1.52
1	A	25	HIS	CG-CD2	6.44	1.43	1.35
1	A	296	HIS	ND1-CE1	6.25	1.38	1.32
1	A	24	ARG	NE-CZ	6.15	1.39	1.33
1	A	296	HIS	CE1-NE2	6.01	1.38	1.32
1	A	24	ARG	CD-NE	5.61	1.54	1.46
1	A	296	HIS	CG-CD2	5.51	1.42	1.35
1	A	208	HIS	ND1-CE1	5.22	1.37	1.32
1	A	214	HIS	CE1-NE2	5.21	1.37	1.32
1	A	21	GLN	CG-CD	5.02	1.64	1.52

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	THR	N-CA-C	9.29	121.41	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	HIS	CA-CB-CG	-8.71	105.08	113.80
1	A	25	HIS	CA-CB-CG	-8.46	105.34	113.80
1	A	254	ARG	NE-CZ-NH1	7.88	129.38	121.50
1	A	254	ARG	NE-CZ-NH2	-7.70	112.28	119.20
1	A	9	GLN	N-CA-C	7.56	119.16	111.07
1	A	254	ARG	CB-CG-CD	7.52	128.59	111.30
1	A	25	HIS	N-CA-C	7.46	119.49	111.36
1	A	40	ASN	CA-CB-CG	-7.19	105.41	112.60
1	A	289	ASP	N-CA-C	7.17	120.14	111.82
1	A	137	ASP	N-CA-C	7.12	119.04	111.28
1	A	24	ARG	CD-NE-CZ	7.10	134.34	124.40
1	A	141	LYS	CB-CG-CD	-7.07	95.04	111.30
1	A	272	LEU	CA-C-O	7.04	128.21	120.82
1	A	10	ILE	N-CA-C	6.87	117.01	110.42
1	A	130	GLU	CB-CA-C	-6.85	96.00	110.31
1	A	254	ARG	CD-NE-CZ	6.84	133.98	124.40
1	A	132	GLU	CA-CB-CG	6.65	127.40	114.10
1	A	290	GLN	N-CA-C	6.50	118.36	111.28
1	A	63	ASP	CA-C-O	6.47	127.79	121.00
1	A	72	ILE	CA-CB-CG1	6.44	121.34	110.40
1	A	21	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	A	236	ASP	CA-C-O	6.30	127.23	120.55
1	A	12	LYS	CA-C-N	-6.30	111.73	122.56
1	A	12	LYS	C-N-CA	-6.30	111.73	122.56
1	A	207	GLU	CA-CB-CG	6.28	126.65	114.10
1	A	23	ILE	N-CA-C	6.25	116.92	110.36
1	A	252	ASP	N-CA-CB	6.24	119.24	109.94
1	A	6	GLU	N-CA-C	6.23	118.07	111.28
1	A	49	VAL	CA-C-O	6.11	126.30	120.31
1	A	118	SER	CB-CA-C	-6.10	97.83	109.66
1	A	157	GLN	CB-CG-CD	-6.00	102.40	112.60
1	A	253	MET	N-CA-C	5.96	117.77	111.28
1	A	41	LYS	CA-C-O	5.93	127.24	120.90
1	A	5	LYS	N-CA-C	5.92	117.73	111.28
1	A	128	LYS	N-CA-C	5.91	118.16	109.24
1	A	28	SER	N-CA-C	5.87	118.74	110.23
1	A	15	SER	N-CA-C	5.83	119.95	112.26
1	A	101	GLU	N-CA-C	5.83	117.63	111.28
1	A	248	LYS	N-CA-C	5.82	117.62	111.28
1	A	166	GLN	N-CA-C	5.79	119.65	112.47
1	A	294	LEU	N-CA-C	5.78	119.15	111.75
1	A	290	GLN	CB-CG-CD	-5.75	102.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	VAL	CA-CB-CG2	5.69	120.07	110.40
1	A	82	ILE	CA-C-N	-5.69	114.18	122.65
1	A	82	ILE	C-N-CA	-5.69	114.18	122.65
1	A	20	TYR	N-CA-C	5.66	117.45	111.28
1	A	237	LYS	CA-C-N	-5.63	113.31	122.26
1	A	237	LYS	C-N-CA	-5.63	113.31	122.26
1	A	62	GLU	N-CA-C	5.60	118.57	111.69
1	A	288	GLN	CA-C-N	-5.58	111.83	120.31
1	A	288	GLN	C-N-CA	-5.58	111.83	120.31
1	A	130	GLU	N-CA-C	5.57	119.34	112.54
1	A	90	ASN	N-CA-C	5.56	120.06	113.16
1	A	270	SER	CB-CA-C	-5.55	101.93	110.81
1	A	21	GLN	CB-CG-CD	5.54	122.03	112.60
1	A	204	LEU	CA-C-O	5.54	126.13	119.43
1	A	127	GLN	CA-C-N	-5.52	113.26	122.21
1	A	127	GLN	C-N-CA	-5.52	113.26	122.21
1	A	189	ALA	N-CA-C	5.52	117.29	111.28
1	A	42	ASN	N-CA-C	5.51	119.71	113.15
1	A	7	PHE	CA-CB-CG	-5.49	108.31	113.80
1	A	283	GLY	CA-C-O	5.49	125.29	119.03
1	A	28	SER	CA-C-O	5.48	127.22	121.19
1	A	33	ARG	NE-CZ-NH2	-5.47	114.27	119.20
1	A	49	VAL	N-CA-C	5.42	116.35	107.24
1	A	103	LYS	CA-C-O	5.42	127.07	120.57
1	A	239	LYS	CB-CA-C	5.32	119.56	111.80
1	A	14	GLY	CA-C-N	-5.31	114.73	122.86
1	A	14	GLY	C-N-CA	-5.31	114.73	122.86
1	A	4	GLU	CA-CB-CG	5.31	124.72	114.10
1	A	156	ARG	CA-C-N	-5.31	115.68	123.00
1	A	156	ARG	C-N-CA	-5.31	115.68	123.00
1	A	205	SER	CA-CB-OG	-5.30	100.50	111.10
1	A	39	LYS	N-CA-C	5.29	118.53	111.75
1	A	100	TRP	N-CA-C	5.29	116.74	110.97
1	A	161	GLU	CA-C-O	5.29	126.14	120.32
1	A	26	GLU	CB-CG-CD	-5.25	103.67	112.60
1	A	114	MET	N-CA-C	5.25	117.28	108.73
1	A	131	LYS	N-CA-C	5.22	117.12	107.73
1	A	76	GLU	CA-CB-CG	5.15	124.40	114.10
1	A	271	TYR	N-CA-C	5.13	116.56	111.07
1	A	63	ASP	N-CA-C	5.12	116.55	110.97
1	A	147	GLU	N-CA-C	5.11	117.57	109.50
1	A	23	ILE	CA-CB-CG1	-5.10	101.73	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	GLN	N-CA-CB	-5.07	102.62	110.57
1	A	7	PHE	N-CA-C	5.06	116.48	110.97
1	A	54	HIS	N-CA-C	5.03	117.65	111.82
1	A	276	GLU	N-CA-C	5.02	116.56	111.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	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	2427	28	2381	24	0
2	A	12	0	9	0	0
3	A	16	0	4	0	0
4	A	241	0	0	2	0
All	All	2696	28	2394	24	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 (24) 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:100:TRP:HE3	1:A:160:LEU:HD13	1.62	0.64
1:A:147:GLU:HB3	1:A:156:ARG:HG2	1.82	0.61
1:A:205:SER:HB3	1:A:207:GLU:OE1	2.00	0.61
1:A:45:ARG:H	1:A:85:GLN:HE22	1.48	0.59
1:A:205:SER:HB3	1:A:207:GLU:CD	2.30	0.56
1:A:238:ARG:HD2	1:A:243:SER:OG	2.10	0.52
1:A:111:ASN:O	1:A:175:HIS:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:H	1:A:85:GLN:NE2	2.09	0.51
1:A:239:LYS:HE2	4:A:386:HOH:O	2.09	0.51
1:A:100:TRP:CZ3	1:A:169:ARG:HG3	2.47	0.50
1:A:112:ARG:HD3	1:A:177:THR:O	2.14	0.48
1:A:23:ILE:HG23	1:A:251:LEU:HD13	1.96	0.47
1:A:10:ILE:HD13	1:A:19:ILE:HG13	1.95	0.47
1:A:6:GLU:O	1:A:10:ILE:HG13	2.16	0.45
1:A:139:ASN:O	1:A:163:LEU:HB2	2.16	0.45
1:A:73:LYS:HD3	4:A:530:HOH:O	2.16	0.44
1:A:83:LEU:HD11	1:A:226:CYS:SG	2.58	0.44
1:A:7:PHE:CZ	1:A:272:LEU:HD13	2.53	0.43
1:A:237:LYS:HB3	1:A:237:LYS:HE2	1.69	0.43
1:A:28:SER:HB3	1:A:30:PHE:CE2	2.54	0.42
1:A:2:GLU:HG3	1:A:4:GLU:H	1.85	0.42
1:A:235:MET:HE3	1:A:235:MET:HB2	1.86	0.42
1:A:227:LEU:HD12	1:A:249:VAL:HG22	2.03	0.41
1:A:17:ALA:O	1:A:21:GLN:HG3	2.21	0.41

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%)	288 (98%)	6 (2%)	1 (0%)	36	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	ILE

5.3.2 Protein sidechains ⓘ

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%)	242 (90%)	28 (10%)	7 1

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	15	SER
1	A	33	ARG
1	A	34	VAL
1	A	49	VAL
1	A	59	LEU
1	A	63	ASP
1	A	71	LEU
1	A	72	ILE
1	A	88	LEU
1	A	128	LYS
1	A	130	GLU
1	A	132	GLU
1	A	140	LEU
1	A	158	LEU
1	A	160	LEU
1	A	163	LEU
1	A	168	THR
1	A	172	LEU
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	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	21	GLN
1	A	61	GLN
1	A	85	GLN
1	A	111	ASN
1	A	123	GLN
1	A	175	HIS
1	A	193	ASN

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 ⓘ

4 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	878	A	301	-	16,16,16	1.29	2 (12%)	19,22,22	1.05	1 (5%)
2	ACT	A	303	-	3,3,3	0.78	0	3,3,3	0.55	0
2	ACT	A	304	-	3,3,3	0.94	0	3,3,3	0.73	0
2	ACT	A	302	-	3,3,3	1.06	0	3,3,3	0.28	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
3	878	A	301	-	-	3/11/12/12	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	878	C14-C16	3.53	1.58	1.54
3	A	301	878	C3-N13	-2.79	1.36	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	878	C5-C4-C3	2.49	121.33	119.09

There are no chirality outliers.

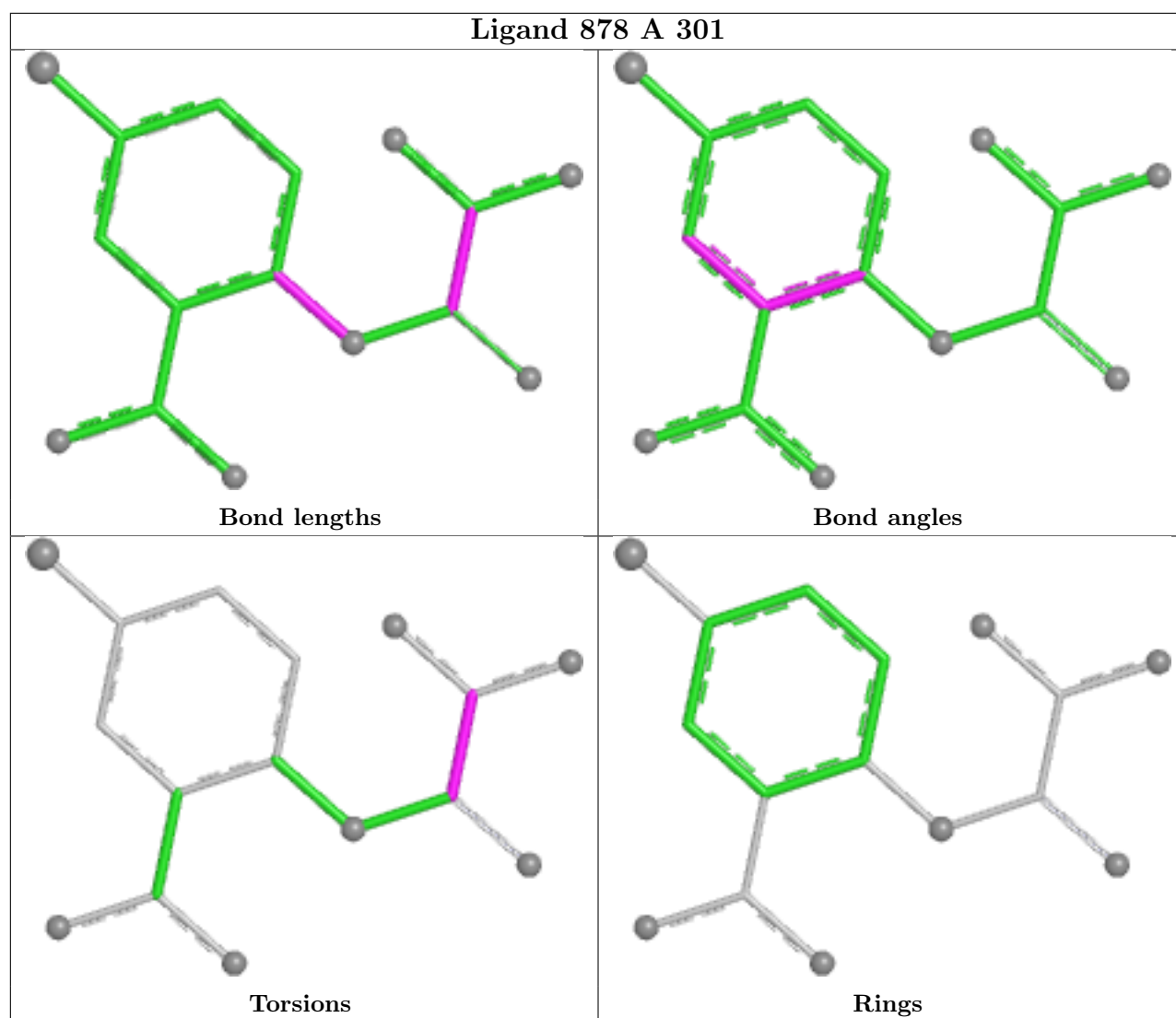
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	878	N13-C14-C16-O17
3	A	301	878	O15-C14-C16-O17
3	A	301	878	O15-C14-C16-O18

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.