



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:48 pm BST

PDB ID : 1C85  
Title : CRYSTAL STRUCTURE OF PROTEIN TYROSINE PHOSPHATASE 1B  
COMPLEXED WITH 2-(OXALYL-AMINO)-BENZOIC ACID  
Authors : Andersen, H.S.; Iversen, L.F.; Branner, S.; Rasmussen, H.B.; Moller, N.P.  
Deposited on : 2000-04-16  
Resolution : 2.72 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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

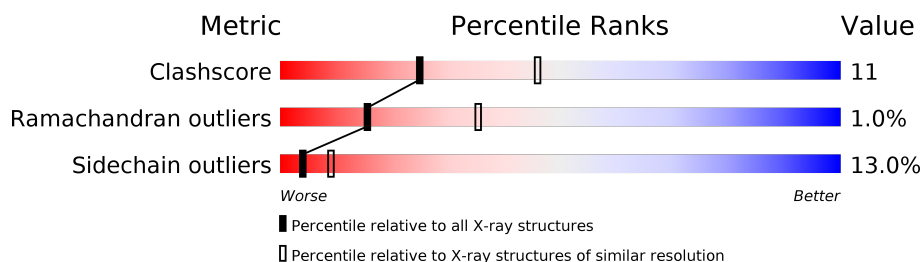
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 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	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)

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	298	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2464 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.

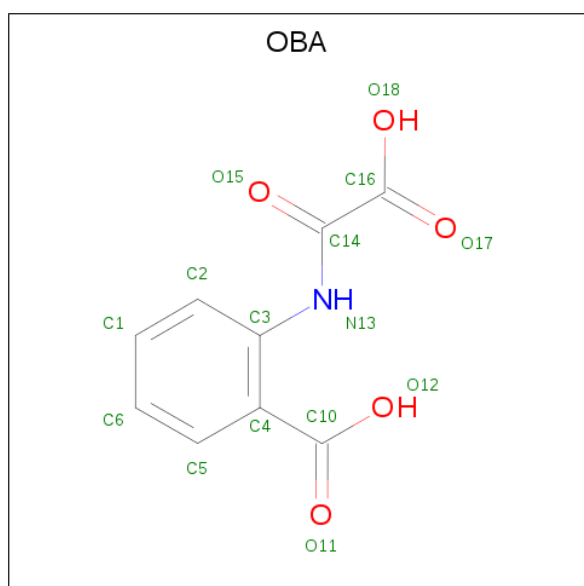
- Molecule 1 is a protein called PROTEIN (PROTEIN-TYROSINE PHOSPHATASE 1B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2426	1535	418	457	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 2-(OXALYL-AMINO)-BENZOIC ACID (three-letter code: OBA) (formula:  $C_9H_7NO_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	9	1	5	0	0

- Molecule 3 is water.

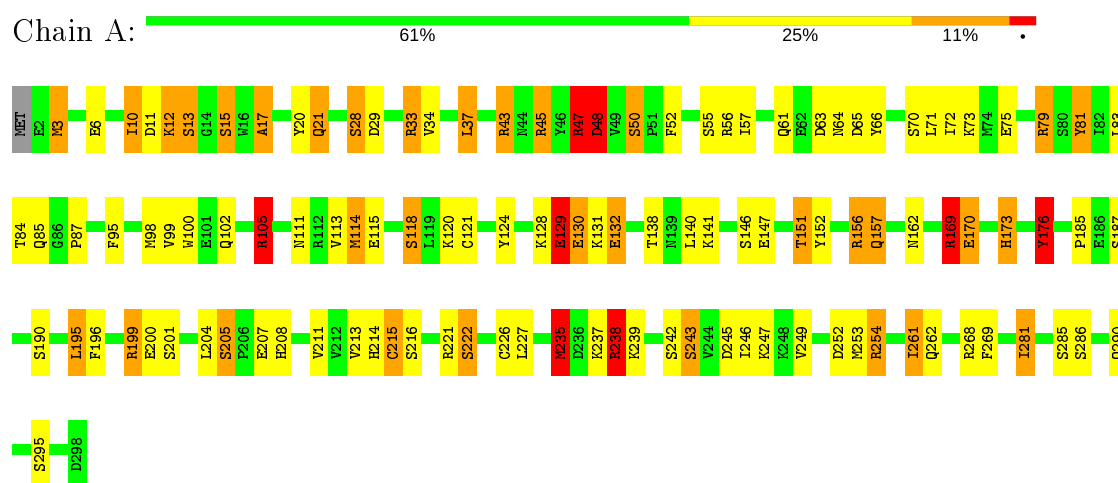
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total 23	O 23	0	0

### 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: 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, $\alpha$ , $\beta$ , $\gamma$	87.87Å 87.87Å 103.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.72	Depositor
% Data completeness (in resolution range)	100.0 (6.00-2.72)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.183 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2464	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 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: OBA

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	1.30	19/2481 (0.8%)	1.78	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	2	9

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	SER	CB-OG	8.43	1.53	1.42
1	A	242	SER	CB-OG	7.39	1.51	1.42
1	A	50	SER	CB-OG	7.34	1.51	1.42
1	A	118	SER	CB-OG	6.50	1.50	1.42
1	A	15	SER	CB-OG	6.04	1.50	1.42
1	A	45	ARG	CZ-NH1	-5.92	1.25	1.33
1	A	55	SER	CB-OG	5.88	1.49	1.42
1	A	243	SER	CB-OG	5.82	1.49	1.42
1	A	21	GLN	CG-CD	5.79	1.64	1.51
1	A	187	SER	CB-OG	5.61	1.49	1.42
1	A	75	GLU	CG-CD	5.57	1.60	1.51
1	A	285	SER	CB-OG	5.51	1.49	1.42
1	A	28	SER	CB-OG	5.48	1.49	1.42
1	A	295	SER	CB-OG	5.39	1.49	1.42
1	A	13	SER	CB-OG	5.36	1.49	1.42
1	A	201	SER	CB-OG	5.26	1.49	1.42
1	A	81	TYR	CE1-CZ	5.22	1.45	1.38
1	A	222	SER	CB-OG	5.22	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ASP	CB-CG	5.04	1.62	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ARG	NE-CZ-NH2	-14.15	113.22	120.30
1	A	33	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	A	56	ARG	NE-CZ-NH1	11.84	126.22	120.30
1	A	105	ARG	NE-CZ-NH1	11.56	126.08	120.30
1	A	47	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	A	105	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	A	221	ARG	NE-CZ-NH2	9.09	124.85	120.30
1	A	199	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	A	141	LYS	CD-CE-NZ	8.56	131.38	111.70
1	A	268	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	79	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	43	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	176	TYR	CB-CG-CD2	7.04	125.22	121.00
1	A	199	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	79	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	238	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	29	ASP	N-CA-CB	-6.39	99.10	110.60
1	A	73	LYS	N-CA-CB	-6.24	99.38	110.60
1	A	253	MET	CG-SD-CE	-6.08	90.47	100.20
1	A	65	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	254	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	48	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	176	TYR	CB-CG-CD1	-5.84	117.49	121.00
1	A	238	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	114	MET	CA-C-N	-5.78	104.49	117.20
1	A	33	ARG	CD-NE-CZ	5.75	131.65	123.60
1	A	157	GLN	CB-CA-C	5.71	121.81	110.40
1	A	254	ARG	CB-CA-C	5.66	121.73	110.40
1	A	132	GLU	CA-C-N	-5.59	104.90	117.20
1	A	130	GLU	CB-CA-C	-5.57	99.25	110.40
1	A	151	THR	CA-CB-CG2	5.55	120.17	112.40
1	A	268	ARG	NH1-CZ-NH2	5.41	125.35	119.40
1	A	129	GLU	C-N-CA	5.33	135.02	121.70
1	A	17	ALA	N-CA-CB	-5.30	102.68	110.10
1	A	45	ARG	N-CA-CB	-5.29	101.07	110.60
1	A	173	HIS	N-CA-CB	-5.29	101.07	110.60
1	A	156	ARG	NH1-CZ-NH2	5.24	125.16	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	GLU	O-C-N	5.20	131.01	122.70
1	A	138	THR	OG1-CB-CG2	5.19	121.94	110.00
1	A	169	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	70	SER	N-CA-CB	-5.14	102.78	110.50
1	A	235	MET	CB-CA-C	5.14	120.67	110.40
1	A	81	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	A	129	GLU	N-CA-CB	-5.10	101.42	110.60
1	A	242	SER	CA-CB-OG	5.08	124.90	111.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	129	GLU	CA
1	A	254	ARG	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	152	TYR	Sidechain
1	A	176	TYR	Sidechain
1	A	20	TYR	Sidechain
1	A	208	HIS	Sidechain
1	A	254	ARG	Sidechain
1	A	47	ARG	Sidechain
1	A	52	PHE	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	2426	0	2381	51	0
2	A	15	0	6	3	0
3	A	23	0	0	0	0
All	All	2464	0	2387	52	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 11.

All (52) 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:34:VAL:HA	1:A:37:LEU:HD22	1.73	0.71
1:A:47:ARG:NH2	1:A:48:ASP:HB3	2.10	0.66
1:A:105:ARG:HH12	1:A:170:GLU:CG	2.08	0.66
1:A:185:PRO:HG2	1:A:269:PHE:CZ	2.30	0.66
1:A:47:ARG:HH22	1:A:48:ASP:HB3	1.59	0.66
1:A:45:ARG:H	1:A:85:GLN:HE22	1.44	0.64
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.62	0.64
1:A:95:PHE:O	1:A:99:VAL:HG23	1.97	0.64
1:A:3:MET:CE	1:A:246:ILE:HD11	2.28	0.63
1:A:87:PRO:HG2	1:A:124:TYR:CD2	2.33	0.63
1:A:235:MET:HG3	1:A:281:ILE:HG21	1.80	0.62
1:A:105:ARG:HH12	1:A:170:GLU:HG2	1.67	0.58
1:A:57:ILE:HD11	1:A:71:LEU:HB2	1.89	0.55
1:A:147:GLU:HB3	1:A:156:ARG:HG2	1.88	0.54
1:A:205:SER:HB3	1:A:207:GLU:OE1	2.09	0.52
1:A:235:MET:CG	1:A:281:ILE:HG21	2.41	0.51
1:A:113:VAL:HG13	1:A:121:CYS:O	2.10	0.51
1:A:111:ASN:HD22	1:A:215:CYS:HA	1.76	0.51
1:A:156:ARG:HB2	1:A:173:HIS:HB3	1.93	0.50
1:A:227:LEU:HD23	1:A:261:ILE:HD11	1.94	0.49
1:A:199:ARG:HG2	1:A:204:LEU:HD12	1.95	0.49
1:A:216:SER:HB3	2:A:301:OBA:O18	2.13	0.49
1:A:61:GLN:HE21	1:A:64:ASN:H	1.60	0.48
1:A:12:LYS:HG2	1:A:13:SER:N	2.28	0.48
1:A:213:VAL:HG12	1:A:222:SER:HB3	1.96	0.48
1:A:115:GLU:HB2	1:A:120:LYS:HG3	1.95	0.47
1:A:195:LEU:HD22	1:A:195:LEU:O	2.13	0.47
1:A:238:ARG:HD2	1:A:243:SER:OG	2.14	0.47
1:A:17:ALA:O	1:A:21:GLN:HG3	2.15	0.47
1:A:105:ARG:HH12	1:A:170:GLU:HG3	1.77	0.46
1:A:105:ARG:CG	1:A:105:ARG:HH11	2.27	0.46
1:A:111:ASN:ND2	1:A:215:CYS:HA	2.31	0.46
1:A:6:GLU:CD	1:A:247:LYS:HZ2	2.18	0.46
1:A:211:VAL:HG13	1:A:213:VAL:HG23	1.98	0.46
1:A:196:PHE:O	1:A:200:GLU:HG2	2.17	0.45
1:A:84:THR:O	1:A:214:HIS:HB2	2.17	0.45
1:A:216:SER:HB3	2:A:301:OBA:H18	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TRP:CZ3	1:A:169:ARG:HG3	2.53	0.44
1:A:43:ARG:NH1	1:A:66:TYR:O	2.50	0.43
2:A:301:OBA:O15	2:A:301:OBA:H2	2.18	0.43
1:A:238:ARG:CD	1:A:243:SER:OG	2.67	0.43
1:A:286:SER:O	1:A:290:GLN:HG3	2.18	0.43
1:A:6:GLU:O	1:A:10:ILE:HG12	2.18	0.43
1:A:3:MET:HE2	1:A:246:ILE:HD11	2.02	0.42
1:A:227:LEU:HD23	1:A:261:ILE:CD1	2.48	0.42
1:A:262:GLN:HA	1:A:262:GLN:NE2	2.34	0.42
1:A:245:ASP:O	1:A:249:VAL:HG23	2.20	0.42
1:A:140:LEU:HD23	1:A:162:ASN:HA	2.02	0.42
1:A:98:MET:O	1:A:102:GLN:HG2	2.20	0.41
1:A:238:ARG:HG2	1:A:238:ARG:H	1.68	0.41
1:A:83:LEU:HD21	1:A:226:CYS:SG	2.60	0.41
1:A:235:MET:O	1:A:239:LYS:N	2.51	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%)	270 (92%)	22 (8%)	3 (1%)	15	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	GLU
1	A	63	ASP
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%)	235 (87%)	35 (13%)	<b>4</b> <b>9</b>

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	10	ILE
1	A	11	ASP
1	A	12	LYS
1	A	15	SER
1	A	28	SER
1	A	33	ARG
1	A	37	LEU
1	A	47	ARG
1	A	48	ASP
1	A	50	SER
1	A	72	ILE
1	A	81	TYR
1	A	105	ARG
1	A	114	MET
1	A	118	SER
1	A	128	LYS
1	A	129	GLU
1	A	130	GLU
1	A	131	LYS
1	A	132	GLU
1	A	146	SER
1	A	151	THR
1	A	157	GLN
1	A	169	ARG
1	A	170	GLU
1	A	176	TYR
1	A	190	SER
1	A	195	LEU
1	A	215	CYS

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Mol	Chain	Res	Type
1	A	235	MET
1	A	237	LYS
1	A	238	ARG
1	A	252	ASP
1	A	281	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	85	GLN
1	A	111	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 carbohydrates 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	OBA	A	301	-	10,15,15	1.35	2 (20%)	12,20,20	1.49	2 (16%)

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	OBA	A	301	-	-	0/4/12/12	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	OBA	C3-N13	-3.22	1.35	1.41
2	A	301	OBA	O15-C14	2.06	1.27	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	OBA	C16-C14-N13	-3.72	109.76	113.74
2	A	301	OBA	C5-C4-C3	2.62	120.56	117.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	OBA	3	0

## 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.