



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:33 PM UTC

PDB ID : 1C84 / pdb_00001c84
Title : CRYSTAL STRUCTURE OF PROTEIN TYROSINE PHOSPHATASE 1B
COMPLEXED WITH 3-(OXALYL-AMINO)-NAPHTHALENE-2-CARBOX
LIC ACID
Authors : Andersen, H.S.; Iversen, L.F.; Branner, S.; Rasmussen, H.B.; Moller, N.P.
Deposited on : 2000-04-14
Resolution : 2.35 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

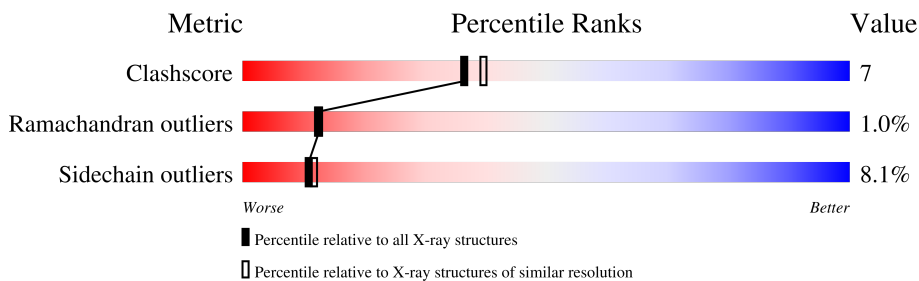
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

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	 59% 30% 9%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2555 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.

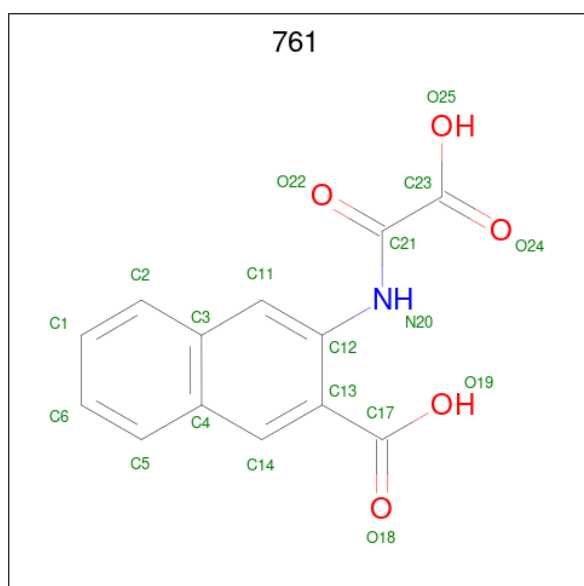
- Molecule 1 is a protein called PROTEIN (PROTEIN-TYROSINE PHOSPHATASE 1B).

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 3-(OXALYL-AMINO)-NAPHTHALENE-2-CARBOXYLIC ACID (CCD ID: 761) (formula: C₁₃H₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	19	13	1	5	0	0

- Molecule 3 is water.

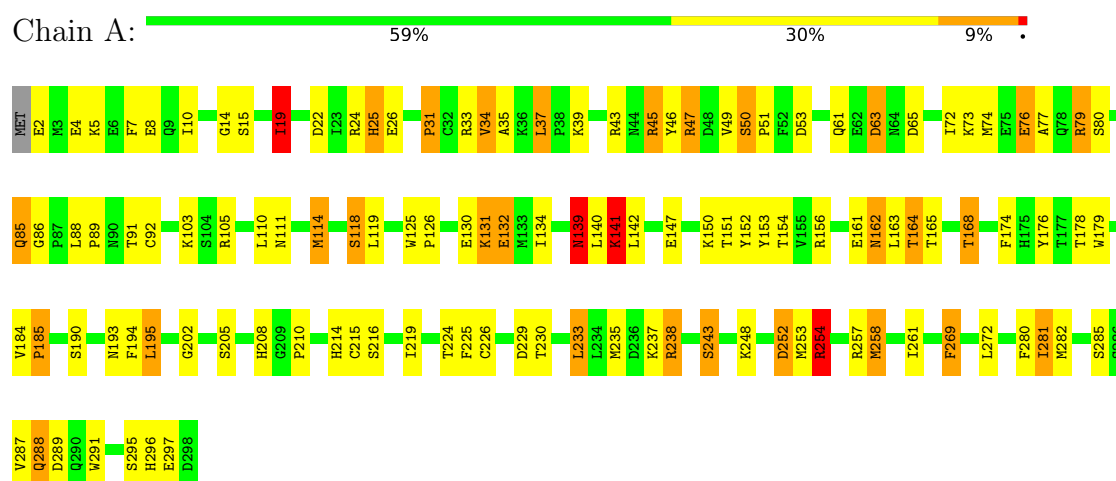
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total 110	O 110	0	0

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)



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	88.03Å 88.03Å 103.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.35	Depositor
% Data completeness (in resolution range)	88.1 (6.00-2.35)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.181 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2555	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: 761

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	1.63	19/2481 (0.8%)	2.04	87/3345 (2.6%)

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	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	LYS	CA-C	7.28	1.63	1.52
1	A	297	GLU	CA-C	6.88	1.61	1.52
1	A	281	ILE	CA-C	6.66	1.61	1.52
1	A	194	PHE	CA-C	6.39	1.61	1.52
1	A	152	TYR	C-N	6.01	1.40	1.33
1	A	156	ARG	CZ-NH2	-5.87	1.25	1.33
1	A	125	TRP	C-N	5.85	1.40	1.33
1	A	254	ARG	CA-C	5.55	1.60	1.52
1	A	296	HIS	CG-CD2	5.54	1.42	1.35
1	A	225	PHE	CA-C	5.42	1.59	1.52
1	A	216	SER	CA-C	5.32	1.59	1.52
1	A	185	PRO	CA-C	5.27	1.59	1.52
1	A	19	ILE	CA-C	5.25	1.59	1.52
1	A	118	SER	CB-OG	5.20	1.52	1.42
1	A	25	HIS	CG-CD2	5.19	1.41	1.35
1	A	224	THR	CB-OG1	5.19	1.52	1.43
1	A	34	VAL	CA-C	5.07	1.59	1.52
1	A	153	TYR	N-CA	5.03	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	SER	CB-OG	5.02	1.52	1.42

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	CYS	CB-CA-C	-10.90	100.78	114.40
1	A	63	ASP	CA-CB-CG	-7.97	104.63	112.60
1	A	297	GLU	N-CA-CB	7.70	121.56	110.16
1	A	164	THR	CA-CB-OG1	7.58	120.97	109.60
1	A	214	HIS	CB-CG-CD2	-7.46	121.51	131.20
1	A	139	ASN	CA-CB-CG	7.31	119.91	112.60
1	A	63	ASP	N-CA-C	7.21	118.92	111.14
1	A	282	MET	N-CA-CB	-7.01	100.89	110.56
1	A	280	PHE	CA-CB-CG	-7.00	106.81	113.80
1	A	168	THR	CA-CB-OG1	-6.97	99.14	109.60
1	A	184	VAL	N-CA-CB	-6.88	107.09	111.83
1	A	178	THR	N-CA-CB	-6.69	101.84	111.54
1	A	25	HIS	CA-C-N	6.62	130.37	120.31
1	A	25	HIS	C-N-CA	6.62	130.37	120.31
1	A	73	LYS	N-CA-CB	-6.59	99.33	110.46
1	A	65	ASP	CA-CB-CG	6.44	119.04	112.60
1	A	50	SER	CA-C-N	6.42	126.64	119.90
1	A	50	SER	C-N-CA	6.42	126.64	119.90
1	A	238	ARG	CD-NE-CZ	-6.42	115.41	124.40
1	A	193	ASN	CB-CG-ND2	6.35	125.92	116.40
1	A	80	SER	N-CA-CB	-6.34	99.83	111.37
1	A	193	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	A	269	PHE	CA-CB-CG	-6.22	107.58	113.80
1	A	289	ASP	CA-C-O	6.21	127.90	121.07
1	A	26	GLU	CB-CG-CD	-6.16	102.13	112.60
1	A	285	SER	CA-CB-OG	6.16	123.42	111.10
1	A	257	ARG	CD-NE-CZ	6.13	132.98	124.40
1	A	168	THR	OG1-CB-CG2	6.06	121.41	109.30
1	A	185	PRO	CB-CA-C	6.03	118.85	110.95
1	A	161	GLU	CA-C-O	6.00	126.72	120.30
1	A	252	ASP	CA-CB-CG	-5.97	106.63	112.60
1	A	63	ASP	N-CA-CB	-5.96	101.43	110.07
1	A	86	GLY	O-C-N	5.95	127.72	121.77
1	A	85	GLN	CA-C-N	-5.90	112.60	121.87
1	A	85	GLN	C-N-CA	-5.90	112.60	121.87
1	A	50	SER	O-C-N	5.85	126.03	121.88
1	A	243	SER	N-CA-CB	-5.79	100.70	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	GLU	N-CA-C	5.76	118.51	111.82
1	A	208	HIS	CA-CB-CG	-5.75	108.05	113.80
1	A	150	LYS	CB-CA-C	5.75	120.06	109.71
1	A	35	ALA	O-C-N	5.75	128.21	122.12
1	A	154	THR	OG1-CB-CG2	-5.72	97.86	109.30
1	A	151	THR	CB-CA-C	-5.69	101.71	110.81
1	A	243	SER	CB-CA-C	-5.68	99.11	110.42
1	A	139	ASN	CB-CA-C	5.68	119.08	111.82
1	A	111	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	24	ARG	CA-C-N	5.62	132.27	121.54
1	A	24	ARG	C-N-CA	5.62	132.27	121.54
1	A	125	TRP	CB-CA-C	5.62	117.58	108.87
1	A	174	PHE	CA-CB-CG	-5.60	108.20	113.80
1	A	130	GLU	CB-CA-C	-5.53	98.76	110.31
1	A	114	MET	CA-C-O	5.52	126.39	120.32
1	A	151	THR	N-CA-CB	-5.47	101.78	109.94
1	A	202	GLY	CA-C-N	-5.47	110.91	121.58
1	A	202	GLY	C-N-CA	-5.47	110.91	121.58
1	A	132	GLU	N-CA-CB	5.44	118.04	110.26
1	A	195	LEU	CA-C-O	5.44	126.31	120.55
1	A	43	ARG	CA-C-N	-5.42	115.34	122.99
1	A	43	ARG	C-N-CA	-5.42	115.34	122.99
1	A	110	LEU	N-CA-CB	-5.40	102.36	110.73
1	A	162	ASN	CB-CA-C	5.35	120.10	111.05
1	A	165	THR	CB-CA-C	-5.34	100.36	109.65
1	A	288	GLN	CB-CA-C	5.33	119.90	110.85
1	A	39	LYS	N-CA-C	5.32	119.25	112.34
1	A	10	ILE	N-CA-C	5.28	115.49	110.53
1	A	80	SER	CA-CB-OG	5.27	121.65	111.10
1	A	119	LEU	CA-C-O	5.25	126.20	120.58
1	A	230	THR	OG1-CB-CG2	-5.24	98.81	109.30
1	A	147	GLU	N-CA-C	5.23	117.14	109.24
1	A	296	HIS	CA-C-N	-5.22	112.88	120.29
1	A	296	HIS	C-N-CA	-5.22	112.88	120.29
1	A	47	ARG	CD-NE-CZ	-5.21	117.11	124.40
1	A	76	GLU	CA-CB-CG	-5.20	103.69	114.10
1	A	31	PRO	CB-CA-C	5.16	118.11	111.56
1	A	91	THR	CA-CB-OG1	5.13	117.30	109.60
1	A	229	ASP	N-CA-C	5.13	117.27	111.11
1	A	258	MET	N-CA-C	5.12	117.32	110.35
1	A	229	ASP	CA-CB-CG	-5.12	107.48	112.60
1	A	49	VAL	O-C-N	5.09	127.97	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	PRO	N-CA-CB	5.09	108.07	103.34
1	A	51	PRO	CB-CA-C	-5.08	105.31	111.46
1	A	254	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	A	45	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	A	233	LEU	CA-C-O	5.07	125.93	120.55
1	A	215	CYS	CA-CB-SG	5.06	126.04	114.40
1	A	25	HIS	CA-CB-CG	5.01	118.81	113.80
1	A	141	LYS	CG-CD-CE	5.01	122.81	111.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	25	HIS	CA
1	A	254	ARG	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	ARG	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	35	0
2	A	19	0	8	1	0
3	A	110	0	0	2	0
All	All	2555	0	2389	35	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 7.

All (35) 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:226:CYS:CB	1:A:253:MET:HE1	2.19	0.72
1:A:226:CYS:HB3	1:A:253:MET:HE1	1.73	0.71
1:A:7:PHE:CZ	1:A:272:LEU:HD21	2.30	0.67
1:A:34:VAL:HA	1:A:37:LEU:HD22	1.79	0.65
1:A:45:ARG:H	1:A:85:GLN:HE22	1.51	0.58
1:A:140:LEU:HD23	1:A:162:ASN:HA	1.86	0.56
1:A:74:MET:HB2	1:A:79:ARG:O	2.07	0.55
1:A:235:MET:HG3	1:A:281:ILE:HG21	1.90	0.52
1:A:238:ARG:HD2	1:A:243:SER:OG	2.10	0.52
1:A:2:GLU:HG3	1:A:4:GLU:H	1.75	0.52
1:A:103:LYS:NZ	3:A:404:HOH:O	2.43	0.51
1:A:19:ILE:O	1:A:22:ASP:HB2	2.11	0.50
1:A:105:ARG:HH11	1:A:105:ARG:HG3	1.78	0.49
1:A:141:LYS:HB2	1:A:163:LEU:HD21	1.94	0.48
1:A:105:ARG:HG3	1:A:105:ARG:NH1	2.31	0.46
1:A:31:PRO:HB3	1:A:33:ARG:HD2	1.98	0.45
1:A:88:LEU:HB3	1:A:89:PRO:HD2	1.98	0.45
1:A:33:ARG:N	1:A:53:ASP:OD2	2.50	0.45
1:A:126:PRO:HD3	1:A:142:LEU:HD23	1.98	0.44
1:A:226:CYS:HB2	1:A:253:MET:HE1	1.95	0.44
1:A:139:ASN:O	1:A:139:ASN:ND2	2.51	0.44
1:A:162:ASN:OD1	1:A:164:THR:HB	2.18	0.43
1:A:176:TYR:CE1	1:A:179:TRP:HB2	2.54	0.43
1:A:45:ARG:H	1:A:85:GLN:NE2	2.15	0.43
1:A:185:PRO:HG2	1:A:269:PHE:CZ	2.54	0.43
1:A:76:GLU:CD	1:A:238:ARG:HH21	2.26	0.42
1:A:50:SER:O	1:A:258:MET:HE3	2.19	0.42
1:A:46:TYR:O	1:A:47:ARG:C	2.62	0.42
1:A:131:LYS:CA	1:A:131:LYS:HE2	2.50	0.41
1:A:176:TYR:CD1	1:A:179:TRP:HB2	2.55	0.41
1:A:92:CYS:SG	3:A:306:HOH:O	2.36	0.41
1:A:61:GLN:HE21	1:A:63:ASP:HB3	1.86	0.41
1:A:291:TRP:O	1:A:295:SER:HB3	2.20	0.41
1:A:219:ILE:HD11	2:A:301:761:H21	2.03	0.41
1:A:77:ALA:HB1	1:A:233:LEU:HD23	2.03	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%)	271 (92%)	21 (7%)	3 (1%)	12	12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	GLY
1	A	261	ILE
1	A	19	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%)	248 (92%)	22 (8%)	11	12

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	8	GLU
1	A	15	SER
1	A	25	HIS
1	A	37	LEU
1	A	72	ILE
1	A	114	MET
1	A	118	SER

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Mol	Chain	Res	Type
1	A	131	LYS
1	A	132	GLU
1	A	134	ILE
1	A	139	ASN
1	A	141	LYS
1	A	168	THR
1	A	190	SER
1	A	195	LEU
1	A	237	LYS
1	A	248	LYS
1	A	252	ASP
1	A	254	ARG
1	A	287	VAL
1	A	288	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	60	HIS
1	A	61	GLN
1	A	85	GLN
1	A	111	ASN
1	A	139	ASN
1	A	262	GLN
1	A	296	HIS

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	761	A	301	-	20,20,20	1.42	3 (15%)	25,28,28	0.99	2 (8%)

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	761	A	301	-	-	3/11/12/12	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	761	C12-N20	-2.87	1.36	1.41
2	A	301	761	C21-C23	2.56	1.57	1.54
2	A	301	761	O25-C23	2.50	1.37	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	761	C5-C4-C14	-2.53	117.66	122.00
2	A	301	761	C14-C4-C3	2.20	122.01	118.96

There are no chirality outliers.

All (3) torsion outliers are listed below:

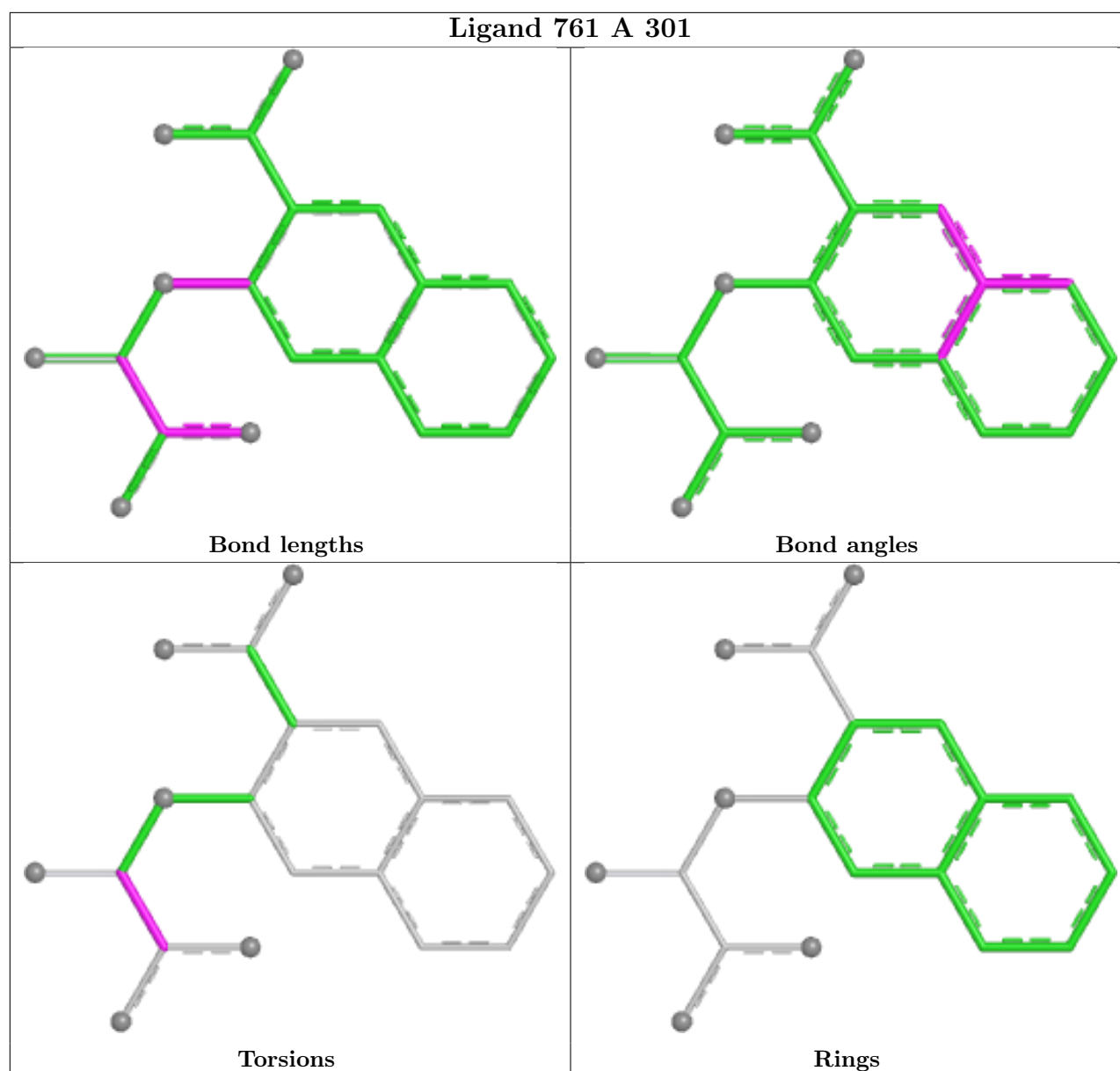
Mol	Chain	Res	Type	Atoms
2	A	301	761	N20-C21-C23-O24
2	A	301	761	O22-C21-C23-O24
2	A	301	761	O22-C21-C23-O25

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	761	1	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.