



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 02:50 pm BST

PDB ID : 1NT1
Title : thrombin in complex with selective macrocyclic inhibitor
Authors : Nantermet, P.G.; Barrow, J.C.; Newton, C.L.; Pellicore, J.M.; Young, M.; Lewis, S.D.; Lucas, B.J.; Krueger, J.A.; McMasters, D.R.; Yan, Y.; Kuo, L.C.; Vacca, J.P.; Selnick, H.G.
Deposited on : 2003-01-28
Resolution : 2.00 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)
Xtrriage (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) : 2.11

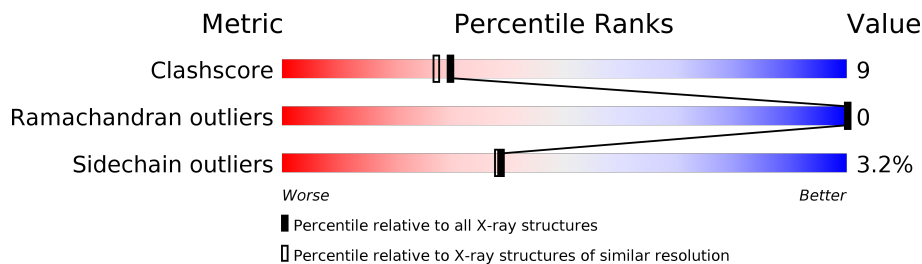
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 ≥ 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	287	
2	H	11	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2506 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 thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2232	1421	392	404	15	0	0	0

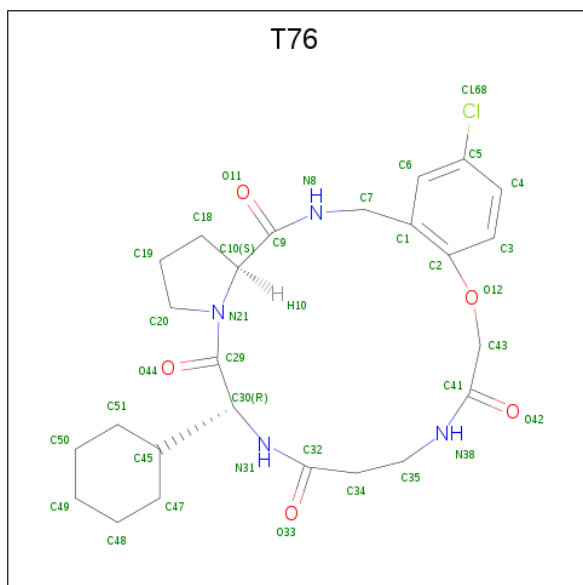
- Molecule 2 is a protein called Hirudin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	11	96	60	11	24	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	362	ALA	GLU	CONFLICT	UNP P28504
H	365	ALA	GLN	CONFLICT	UNP P28504

- Molecule 3 is (6R,21AS)-17-CHLORO-6-CYCLOHEXYL-2,3,6,7,10,11,19,20-OCTAHYDR O-1H,5H-PYRROLO[1,2-K][1,4,8,11,14]BENZOXATETRAAZA-CYCLOHEPTADECINE-5,8,12,21(9H,13H,21AH)-TETRONE (three-letter code: T76) (formula: C₂₅H₃₃ClN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	35	25	1	4	5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	141	Total	O	0	0
			141	141		
4	H	2	Total	O	0	0
			2	2		

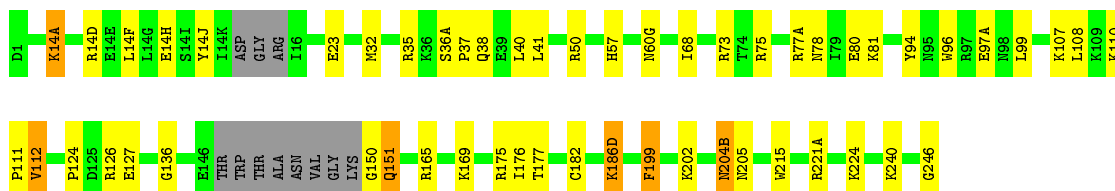
3 Residue-property plots [i](#)

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.

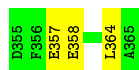
- Molecule 1: thrombin

Chain A:  77% 17%



- Molecule 2: Hirudin

Chain H:  73% 27%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.10Å 72.10Å 73.20Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2506	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: T76, TYS

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	0.48	0/2286	0.74	1/3084 (0.0%)
2	H	0.53	0/80	0.62	0/105
All	All	0.48	0/2366	0.74	1/3189 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	PHE	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2232	0	2197	43	0
2	H	96	0	76	3	0
3	A	35	0	33	1	0
4	A	141	0	0	5	0
4	H	2	0	0	0	0
All	All	2506	0	2306	44	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 9.

All (44) 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:14(A):LYS:HE3	1:A:23:GLU:HG3	1.69	0.74
1:A:75:ARG:HH11	2:H:357:GLU:HB2	1.55	0.69
1:A:38:GLN:HE22	2:H:364:LEU:HD21	1.63	0.64
1:A:221(A):ARG:HB2	1:A:224:LYS:HB2	1.79	0.63
1:A:35:ARG:O	1:A:38:GLN:HA	1.98	0.63
1:A:169:LYS:HA	1:A:176:ILE:HD12	1.83	0.61
1:A:186(D):LYS:HB2	1:A:186(D):LYS:NZ	2.18	0.59
2:H:358:GLU:H	2:H:358:GLU:CD	2.08	0.56
1:A:32:MET:HG3	1:A:40:LEU:CD1	2.38	0.54
1:A:50:ARG:NE	1:A:108:LEU:O	2.41	0.53
1:A:80:GLU:O	1:A:81:LYS:HD3	2.09	0.52
1:A:110:LYS:HD3	1:A:111:PRO:CD	2.41	0.51
1:A:127:GLU:CD	1:A:127:GLU:H	2.15	0.51
1:A:110:LYS:HD3	1:A:111:PRO:HD2	1.92	0.51
1:A:35:ARG:HB2	1:A:41:LEU:HD21	1.92	0.50
1:A:136:GLY:HA3	1:A:199:PHE:CZ	2.47	0.50
1:A:204(B):ASN:C	1:A:204(B):ASN:HD22	2.12	0.49
1:A:165:ARG:HG3	4:A:677:HOH:O	2.12	0.49
1:A:186(D):LYS:HB2	1:A:186(D):LYS:HZ3	1.79	0.48
1:A:221(A):ARG:NH1	4:A:915:HOH:O	2.46	0.47
1:A:57:HIS:CD2	3:A:247:T76:H181	2.50	0.47
1:A:73:ARG:HD2	4:A:660:HOH:O	2.15	0.46
1:A:99:LEU:HD12	1:A:215:TRP:HB3	1.98	0.46
1:A:77(A):ARG:O	1:A:78:ASN:HB2	2.16	0.44
1:A:151:GLN:OE1	1:A:151:GLN:N	2.49	0.44
1:A:14(D):ARG:NH2	1:A:14(H):GLU:HG2	2.32	0.44
1:A:75:ARG:HA	1:A:75:ARG:HD3	1.79	0.44
1:A:126:ARG:HB3	1:A:127:GLU:OE1	2.18	0.44
1:A:169:LYS:HE2	1:A:176:ILE:HB	2.01	0.43
1:A:50:ARG:NH1	1:A:107:LYS:HE3	2.34	0.43
1:A:240:LYS:HB2	1:A:240:LYS:HE3	1.84	0.43
1:A:110:LYS:HA	1:A:111:PRO:HD3	1.91	0.43
1:A:36(A):SER:HA	1:A:37:PRO:C	2.36	0.43
1:A:150:GLY:N	4:A:779:HOH:O	2.52	0.42
1:A:68:ILE:HD12	1:A:112:VAL:HG11	2.01	0.41
1:A:73:ARG:CZ	1:A:151:GLN:HB2	2.50	0.41
1:A:14(J):TYR:HE2	1:A:202:LYS:O	2.03	0.41
1:A:107:LYS:NZ	1:A:246:GLY:O	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:NH2	1:A:177:THR:O	2.53	0.41
1:A:204(B):ASN:HD22	1:A:205:ASN:N	2.19	0.41
1:A:127:GLU:CD	1:A:127:GLU:N	2.73	0.41
1:A:97(A):GLU:OE2	1:A:175:ARG:NH1	2.53	0.41
1:A:60(G):ASN:ND2	4:A:889:HOH:O	2.53	0.40
1:A:94:TYR:CZ	1:A:96:TRP:HB3	2.56	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	270/287 (94%)	260 (96%)	10 (4%)	0	100	100
2	H	8/11 (73%)	8 (100%)	0	0	100	100
All	All	278/298 (93%)	268 (96%)	10 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	241/251 (96%)	233 (97%)	8 (3%)	38	37
2	H	8/8 (100%)	8 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	249/259 (96%)	241 (97%)	8 (3%)	39 38

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14(A)	LYS
1	A	14(F)	LEU
1	A	112	VAL
1	A	124	PRO
1	A	151	GLN
1	A	182	CYS
1	A	186(D)	LYS
1	A	204(B)	ASN

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

Mol	Chain	Res	Type
1	A	30	GLN
1	A	60(G)	ASN
1	A	78	ASN
1	A	156	GLN
1	A	204(B)	ASN
1	A	239	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue 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	TYS	H	363	2	15,16,17	3.43	2 (13%)	18,22,24	1.14	2 (11%)

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	TYS	H	363	2	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	363	TYS	OH-CZ	-10.58	1.25	1.42
2	H	363	TYS	OH-S	-7.75	1.46	1.58

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	363	TYS	OH-S-O2	2.35	114.56	107.71
2	H	363	TYS	O3-S-OH	2.10	110.88	105.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
3	T76	A	247	-	38,38,38	0.83	1 (2%)	51,52,52	1.39	6 (11%)

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	T76	A	247	-	-	0/36/54/54	0/3/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	247	T76	C6-C5	2.43	1.42	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	247	T76	C35-N38-C41	-4.67	114.17	122.84
3	A	247	T76	C43-O12-C2	-4.16	109.00	117.60
3	A	247	T76	C30-N31-C32	-3.34	115.43	121.83
3	A	247	T76	C7-N8-C9	-2.41	118.86	122.34
3	A	247	T76	C35-C34-C32	-2.23	108.64	112.36
3	A	247	T76	C18-C10-N21	-2.06	99.97	103.03

There are no chirality outliers.

There are no torsion outliers.

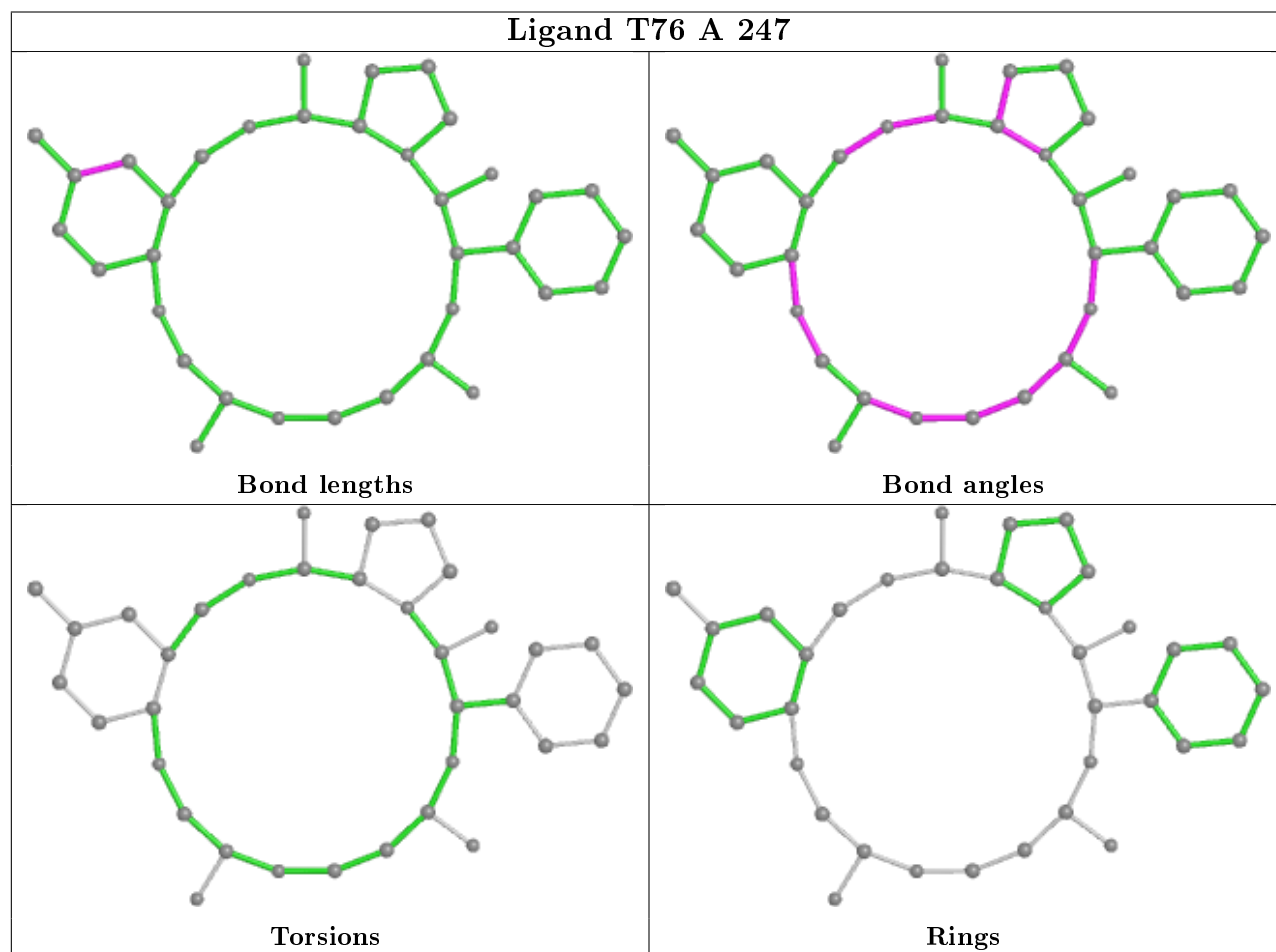
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	247	T76	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.