



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:34 PM UTC

PDB ID : 1AY6 / pdb_00001ay6
Title : THROMBIN INHIBITOR FROM THEONALLA, CYCLOTHEANAMIDE-BASED MACROCYCLIC TRIPEPTIDE MOTIF
Authors : Ganesh, V.; Maryanoff, B.E.; Tulinsky, A.
Deposited on : 1997-11-14
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

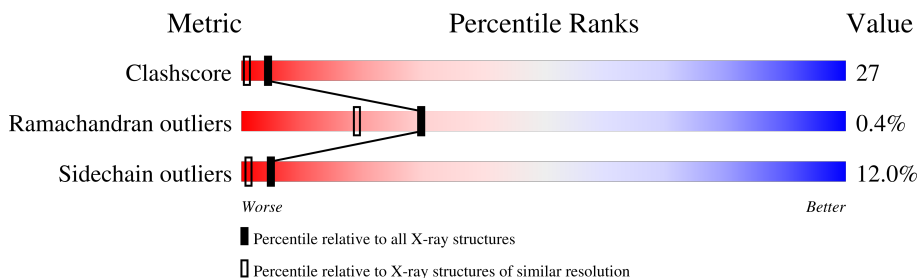
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	L	36	
2	H	259	
3	I	13	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TYS	I	63	-	-	X	-
4	1ZV	H	5	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2568 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 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	29	Total	C	N	O	S	0	0	0
			235	147	38	49	1			

- Molecule 2 is a protein called THROMBIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	252	Total	C	N	O	S	0	0	0
			2030	1294	358	364	14			

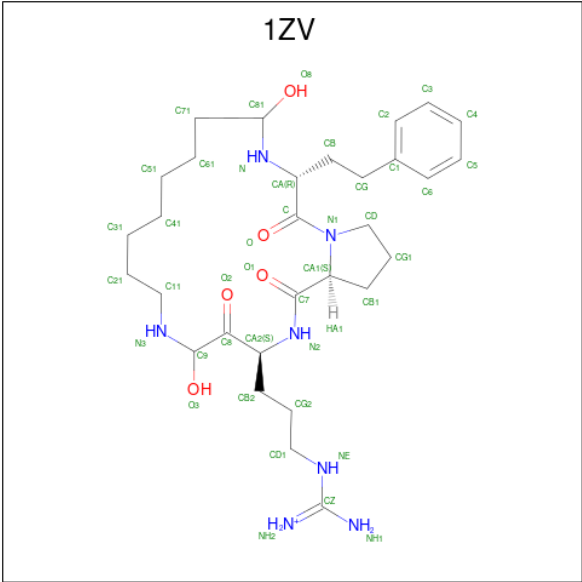
- Molecule 3 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	0	0	0
			85	53	10	21	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	52	ACE	-	insertion	UNP P01050
I	53	ASN	-	insertion	UNP P01050
I	54	GLU	-	insertion	UNP P01050

- Molecule 4 is amino({3-[(3R,5R,14S,16S,21aR)-5,14-dihydroxy-1,4,17-trioxo-16-(2-phenylethyl)icosahydro-1H-pyrrolo[1,2-d][1,4,7,11]tetraazacyclononadecin-3-yl]propyl}amino)methan iminium (CCD ID: 1ZV) (formula: C₃₀H₅₀N₇O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			42	30	7	5		

- Molecule 5 is water.

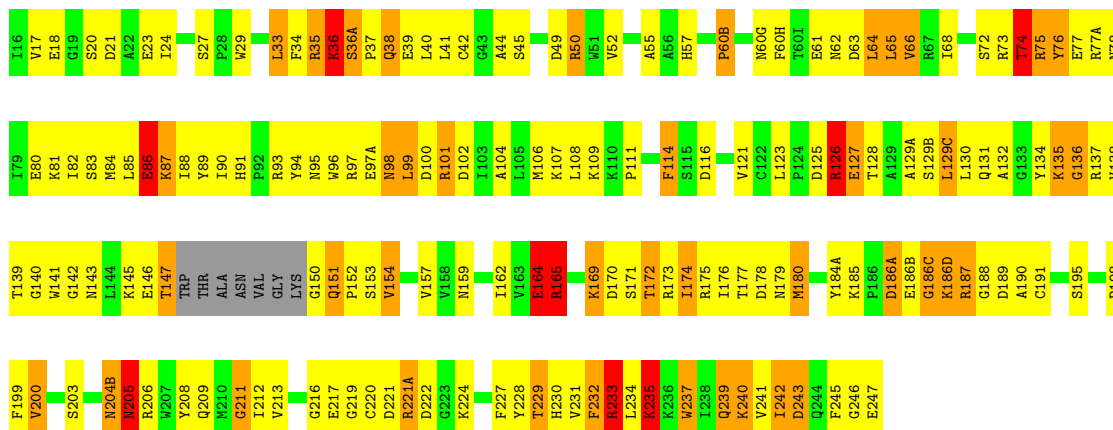
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	15	Total	O	0	0
			15	15		
5	H	160	Total	O	0	0
			160	160		
5	I	1	Total	O	0	0
			1	1		

Note EDS was not executed.

Chain L:



Chain H:



Chain I:



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	71.08Å 72.14Å 72.82Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	7.00 – 1.80	Depositor
% Data completeness (in resolution range)	75.0 (7.00-1.80)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.12	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2568	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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: TYS, 1ZV

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	L	1.44	1/237 (0.4%)	2.82	26/315 (8.3%)
2	H	1.75	22/2082 (1.1%)	2.74	196/2812 (7.0%)
3	I	1.01	0/69	2.45	5/89 (5.6%)
All	All	1.70	23/2388 (1.0%)	2.74	227/3216 (7.1%)

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
2	H	0	3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	211	GLY	N-CA	10.31	1.55	1.45
2	H	78	ASN	N-CA	9.21	1.56	1.46
2	H	200	VAL	N-CA	8.31	1.55	1.46
2	H	137	ARG	NE-CZ	6.99	1.40	1.33
2	H	159	ASN	C-N	-6.90	1.25	1.33

The worst 5 of 227 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	93	ARG	CD-NE-CZ	19.94	152.32	124.40
2	H	243	ASP	CA-CB-CG	14.26	126.86	112.60
2	H	205	ASN	OD1-CG-ND2	12.99	135.59	122.60
2	H	97	ARG	CD-NE-CZ	-12.39	107.05	124.40
2	H	205	ASN	CB-CA-C	12.24	129.67	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	126	ARG	Sidechain
2	H	233	ARG	Sidechain
2	H	77	GLU	Mainchain

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	L	235	0	234	28	0
2	H	2030	0	1992	88	2
3	I	85	0	64	16	1
4	H	42	0	45	2	0
5	H	160	0	0	10	1
5	I	1	0	0	0	0
5	L	15	0	0	4	0
All	All	2568	0	2335	126	2

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 27.

The worst 5 of 126 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:L:14(D):ARG:NH2	1:L:14(H):GLU:OE1	1.73	1.22
1:L:14(D):ARG:HD2	5:L:461:HOH:O	1.47	1.10
2:H:81:LYS:CB	5:H:829:HOH:O	2.02	1.08
1:L:14(D):ARG:HE	1:L:14(H):GLU:HB3	1.19	1.05
1:L:14(D):ARG:CD	5:L:461:HOH:O	2.02	1.04

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:ARG:NH1	3:I:57:GLU:OE2[2_555]	2.06	0.14
2:H:172:THR:O	5:H:422:HOH:O[4_546]	2.10	0.10

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	L	27/36 (75%)	22 (82%)	4 (15%)	1 (4%)	2	0
2	H	248/259 (96%)	238 (96%)	10 (4%)	0	100	100
3	I	7/13 (54%)	6 (86%)	1 (14%)	0	100	100
All	All	282/308 (92%)	266 (94%)	15 (5%)	1 (0%)	30	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1(B)	ALA

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	L	26/31 (84%)	24 (92%)	2 (8%)	12	3
2	H	218/225 (97%)	192 (88%)	26 (12%)	5	1
3	I	7/11 (64%)	5 (71%)	2 (29%)	0	0
All	All	251/267 (94%)	221 (88%)	30 (12%)	5	1

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	129(B)	SER
2	H	243	ASP
2	H	154	VAL
3	I	62	GLU
2	H	239	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	38	GLN
2	H	156	GLN
2	H	204(B)	ASN
2	H	205	ASN
2	H	239	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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
3	TYS	I	63	3	15,16,17	1.64	2 (13%)	15,22,24	1.83	5 (33%)

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	TYS	I	63	3	-	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)
3	I	63	TYS	OH-CZ	-4.54	1.35	1.42
3	I	63	TYS	OH-S	3.22	1.64	1.58

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	63	TYS	CB-CG-CD1	-3.14	115.06	120.90
3	I	63	TYS	CE2-CZ-CE1	2.65	124.03	120.16
3	I	63	TYS	CD1-CE1-CZ	-2.63	116.72	119.73
3	I	63	TYS	CD2-CG-CD1	2.51	121.96	118.23
3	I	63	TYS	O3-S-O1	2.26	116.46	108.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	63	TYS	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
4	1ZV	H	5	2	40,44,44	2.16	6 (15%)	43,57,57	2.39	16 (37%)

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
4	1ZV	H	5	2	2/2/10/14	17/46/61/61	0/2/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	5	1ZV	O2-C8	10.52	1.37	1.21
4	H	5	1ZV	O8-C81	-4.83	1.26	1.40
4	H	5	1ZV	CZ-NE	-2.76	1.28	1.33
4	H	5	1ZV	CA2-C8	2.69	1.56	1.52
4	H	5	1ZV	CA-N	2.52	1.53	1.47

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	5	1ZV	CB-CA-C	6.79	126.58	109.75
4	H	5	1ZV	O8-C81-C71	6.20	123.92	109.17
4	H	5	1ZV	C51-C61-C71	5.20	133.20	113.62
4	H	5	1ZV	C5-C6-C1	3.59	125.65	120.61
4	H	5	1ZV	CB-CG-C1	3.26	123.95	113.22

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	5	1ZV	C9
4	H	5	1ZV	C81

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	5	1ZV	N-CA-CB-CG
4	H	5	1ZV	C-CA-CB-CG
4	H	5	1ZV	CA-CB-CG-C1
4	H	5	1ZV	O2-C8-C9-O3

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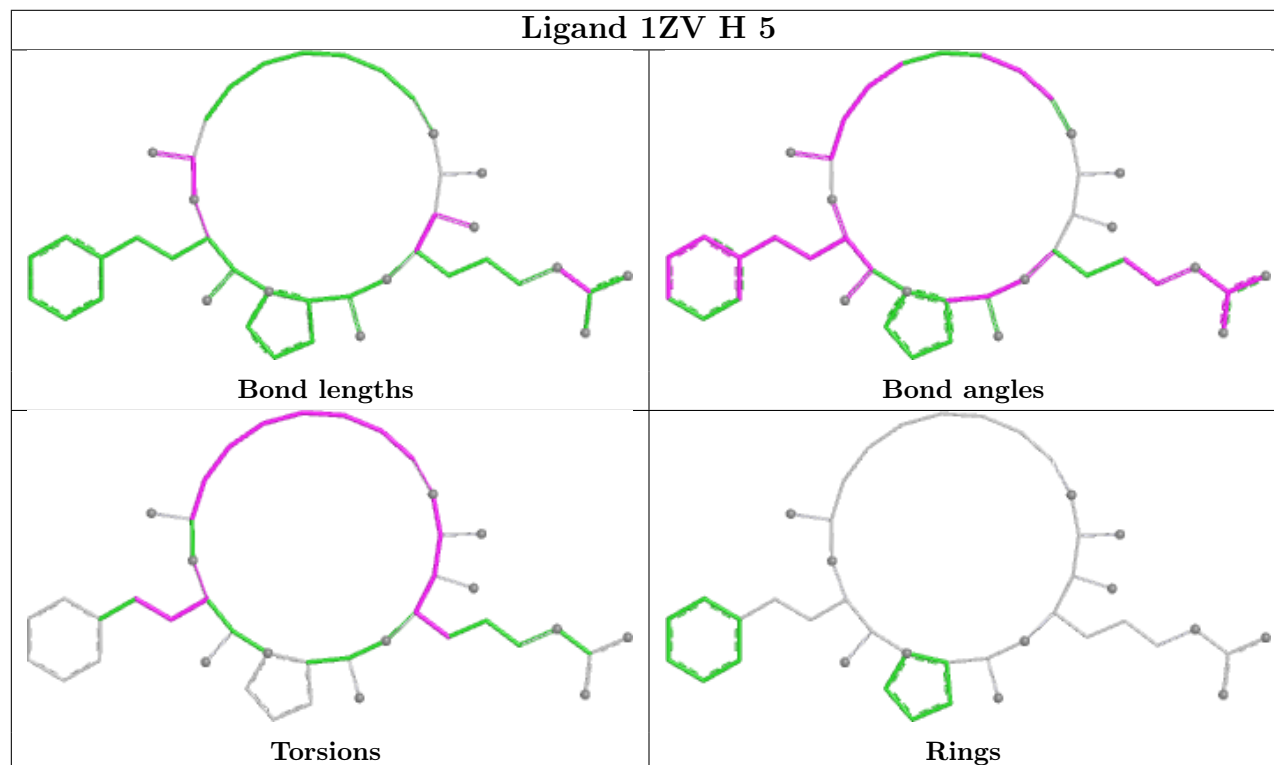
Mol	Chain	Res	Type	Atoms
4	H	5	1ZV	C8-C9-N3-C11

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	5	1ZV	2	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.