



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:30 AM UTC

PDB ID : 2GDE / pdb_00002gde
Title : Thrombin in complex with inhibitor
Authors : Xue, Y.
Deposited on : 2006-03-16
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 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

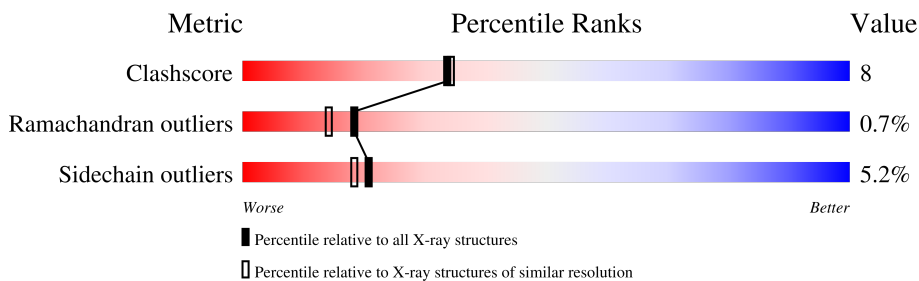
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 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	D	10	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2450 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	27	Total	C	N	O	S	0	0	0
			222	140	36	45	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	249	Total	C	N	O	S	0	0	0
			2014	1283	357	360	14			

- Molecule 3 is a protein called Hirudin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	10	Total	C	N	O	S	0	0	0
			90	56	10	23	1			

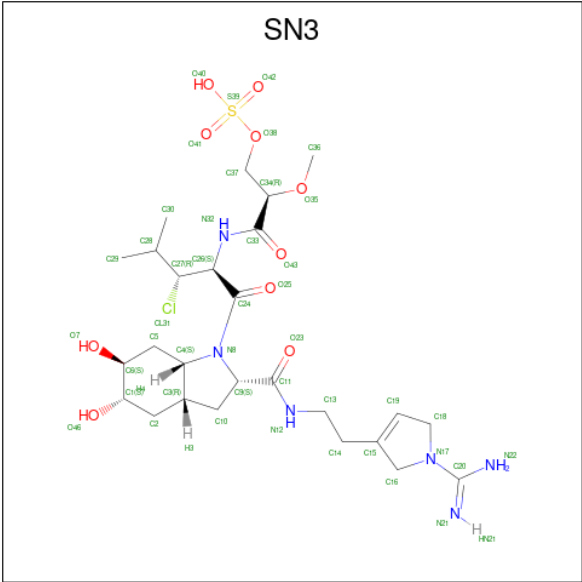
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	361	GLY	GLU	conflict	UNP P28504

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Na	0	0
			1	1		

- Molecule 5 is (R)-3-((2S,3R)-1-((2S,3AR,5S,6S,7AS)-2-(2-(1-CARBAMIMIDOYL-2,5-DIHYDRO-1H-PYRROL-3-YL)ETHYLCARBAMOYL)-5,6-DIHYDROXYOCTA HYDRO-1H-INDOL-1-YL)-3-CHLORO-4-METHYL-1-OXOPENTAN-2-YLAMINO)-2-METHOXY-3-OXOPROPYL HYDROGEN SULFATE (CCD ID: SN3) (formula: C₂₆H₄₃ClN₆O₁₀S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	H	1	Total	C	Cl	N	O	S	0	0
			44	26	1	6	10	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	6	Total	O	0	0
			6	6		
6	H	73	Total	O	0	0
			73	73		

3 Residue-property plots [i](#)

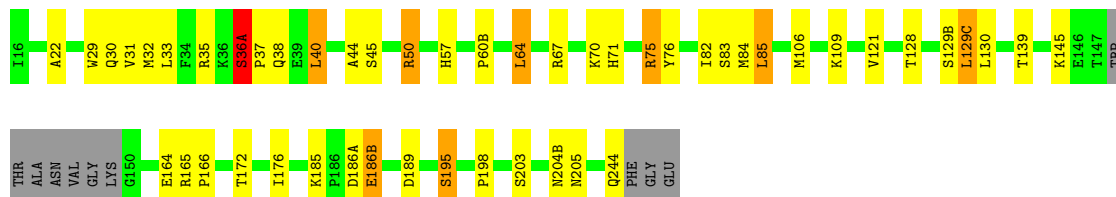
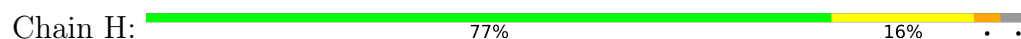
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

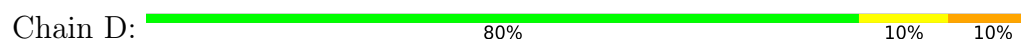
- Molecule 1: Thrombin light chain



- Molecule 2: Thrombin heavy chain



- Molecule 3: Hirudin



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	70.08 Å 72.17 Å 70.36 Å 90.00° 99.06° 90.00°	Depositor
Resolution (Å)	69.50 – 2.00	Depositor
% Data completeness (in resolution range)	97.7 (69.50-2.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2450	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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, NA, SN3

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	0.76	0/224	0.91	0/298
2	H	0.79	0/2065	0.98	5/2790 (0.2%)
3	D	0.65	0/74	0.96	0/96
All	All	0.78	0/2363	0.97	5/3184 (0.2%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	36(A)	SER	CA-C-N	-12.38	104.36	119.84
2	H	36(A)	SER	C-N-CA	-12.38	104.36	119.84
2	H	185	LYS	CA-C-N	5.60	125.96	119.47
2	H	185	LYS	C-N-CA	5.60	125.96	119.47
2	H	60(B)	PRO	N-CA-C	5.43	117.33	110.70

There are no chirality outliers.

There are no planarity outliers.

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	222	0	225	2	0
2	H	2014	0	1992	33	0
3	D	90	0	70	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
5	H	44	0	42	1	0
6	H	73	0	0	3	0
6	L	6	0	0	0	0
All	All	2450	0	2329	36	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 8.

All (36) 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)
2:H:36(A):SER:OG	2:H:37:PRO:HD2	1.66	0.96
2:H:165:ARG:HG3	6:H:451:HOH:O	1.71	0.89
2:H:50:ARG:HD3	6:H:446:HOH:O	1.80	0.81
2:H:36(A):SER:OG	2:H:37:PRO:CD	2.29	0.81
2:H:64:LEU:HD12	2:H:85:LEU:HD11	1.64	0.80
2:H:33:LEU:HD21	2:H:106:MET:HE1	1.66	0.77
2:H:75:ARG:NE	2:H:76:TYR:O	2.18	0.76
2:H:32:MET:HG3	2:H:40:LEU:HD12	1.70	0.73
2:H:84:MET:HE3	2:H:109:LYS:HD2	1.76	0.68
1:L:5:PRO:HA	1:L:9:LYS:HD3	1.83	0.59
2:H:30:GLN:NE2	2:H:139:THR:OG1	2.36	0.59
2:H:75:ARG:CD	2:H:76:TYR:O	2.54	0.55
2:H:186(A):ASP:OD1	2:H:186(B):GLU:N	2.40	0.54
2:H:35:ARG:O	2:H:38:GLN:HA	2.09	0.53
2:H:75:ARG:HD2	2:H:76:TYR:O	2.09	0.52
3:D:363:TYS:O	3:D:364:LEU:HB2	2.10	0.52
2:H:33:LEU:CD2	2:H:106:MET:HE1	2.38	0.52
2:H:172:THR:HG21	2:H:176:ILE:HD11	1.92	0.51
2:H:75:ARG:HD2	2:H:76:TYR:N	2.26	0.51
2:H:75:ARG:CZ	2:H:76:TYR:O	2.59	0.50
2:H:50:ARG:CD	6:H:446:HOH:O	2.51	0.49
2:H:164:GLU:HB3	2:H:166:PRO:HD2	1.97	0.47
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.31	0.46
2:H:31:VAL:HB	2:H:44:ALA:HB3	1.97	0.46
2:H:22:ALA:O	2:H:71:HIS:HE1	2.01	0.44
1:L:14(I):SER:C	1:L:14(K):ILE:H	2.26	0.43
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.25	0.43
2:H:189:ASP:OD1	5:H:401:SN3:N21	2.43	0.42
2:H:70:LYS:HE3	2:H:70:LYS:HB3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:30:GLN:HE22	2:H:198:PRO:HD2	1.85	0.42
2:H:186(A):ASP:OD1	2:H:186(A):ASP:C	2.63	0.41
2:H:57:HIS:CE1	2:H:195:SER:OG	2.73	0.41
2:H:67:ARG:HG2	2:H:82:ILE:HG12	2.02	0.41
2:H:128:THR:HG22	2:H:129(C):LEU:HD12	2.03	0.41
2:H:29:TRP:CG	2:H:121:VAL:HB	2.56	0.41
2:H:45:SER:HB3	2:H:198:PRO:HG3	2.03	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	L	25/36 (69%)	23 (92%)	2 (8%)	0	100	100
2	H	245/259 (95%)	234 (96%)	9 (4%)	2 (1%)	16	11
3	D	7/10 (70%)	7 (100%)	0	0	100	100
All	All	277/305 (91%)	264 (95%)	11 (4%)	2 (1%)	18	14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	36(A)	SER
2	H	186(B)	GLU

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	25/31 (81%)	25 (100%)	0	100	100
2	H	218/225 (97%)	205 (94%)	13 (6%)	17	14
3	D	8/8 (100%)	8 (100%)	0	100	100
All	All	251/264 (95%)	238 (95%)	13 (5%)	21	18

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	40	LEU
2	H	50	ARG
2	H	64	LEU
2	H	75	ARG
2	H	83	SER
2	H	85	LEU
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	130	LEU
2	H	145	LYS
2	H	195	SER
2	H	205	ASN
2	H	244	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	30	GLN
2	H	62	ASN
2	H	71	HIS
2	H	151	GLN
2	H	204(B)	ASN
2	H	209	GLN
2	H	244	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	D	363	3	15,16,17	1.29	2 (13%)	15,22,24	0.82	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	TYS	D	363	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	D	363	TYS	OH-CZ	-3.81	1.36	1.42
3	D	363	TYS	OH-S	-2.79	1.53	1.58

There are no bond angle outliers.

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	D	363	TYS	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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
5	SN3	H	401	-	43,46,46	0.93	1 (2%)	54,67,67	1.68	11 (20%)

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
5	SN3	H	401	-	-	1/42/83/83	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	401	SN3	C6-C1	2.63	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	401	SN3	C19-C18-N17	5.42	105.99	102.03
5	H	401	SN3	O40-S39-O42	4.27	123.51	108.56
5	H	401	SN3	O38-C37-C34	3.22	113.56	107.79
5	H	401	SN3	C13-C14-C15	-3.18	107.98	114.42
5	H	401	SN3	O25-C24-N8	-2.84	117.33	121.63
5	H	401	SN3	C10-C9-N8	2.49	106.60	103.48
5	H	401	SN3	C3-C2-C1	2.48	117.52	113.22
5	H	401	SN3	C10-C3-C2	-2.40	109.57	116.37
5	H	401	SN3	C30-C28-C27	-2.29	107.50	112.19
5	H	401	SN3	C2-C1-C6	2.28	113.19	110.38
5	H	401	SN3	C18-C19-C15	-2.02	110.05	112.32

There are no chirality outliers.

All (1) torsion outliers are listed below:

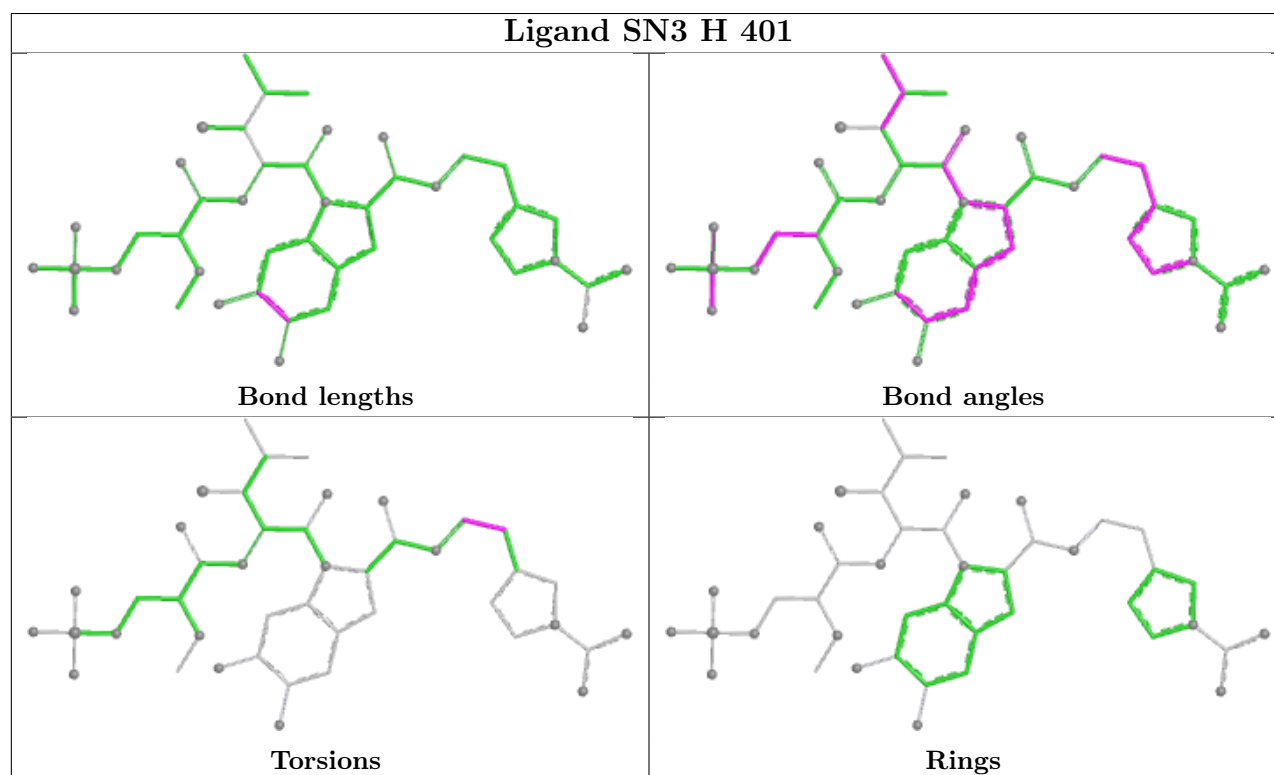
Mol	Chain	Res	Type	Atoms
5	H	401	SN3	N12-C13-C14-C15

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	401	SN3	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.