



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 17, 2018 – 04:26 pm GMT

PDB ID : 1C4U
Title : SELECTIVE NON ELECTROPHILIC THROMBIN INHIBITORS WITH
CYCLOHEXYL MOIETIES.
Authors : Krishnan, R.; Mochalkin, I.; Arni, R.K.; Tulinsky, A.
Deposited on : 1999-09-25
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

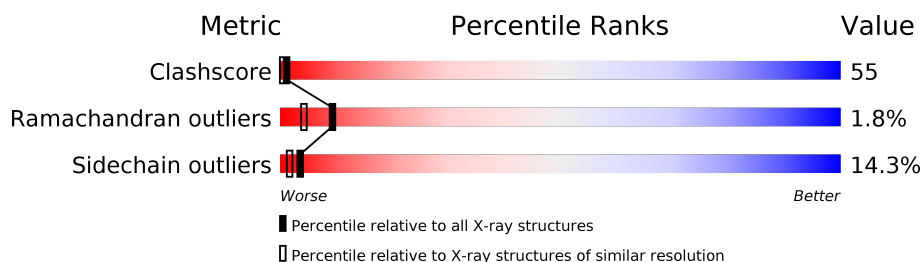
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	122078	5107 (2.10-2.10)
Ramachandran outliers	120005	5057 (2.10-2.10)
Sidechain outliers	119972	5058 (2.10-2.10)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	36	
2	2	259	
3	3	14	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2479 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
1	1	30	Total	C	N	O	S	0	0	0
			240	150	39	50	1			

- Molecule 2 is a protein called thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	252	Total	C	N	O	S	0	0	0
			2039	1299	360	366	14			

- Molecule 3 is a protein called PROTEIN (HIRUGEN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	8	Total	C	N	O	S	0	0	0
			68	43	8	16	1			

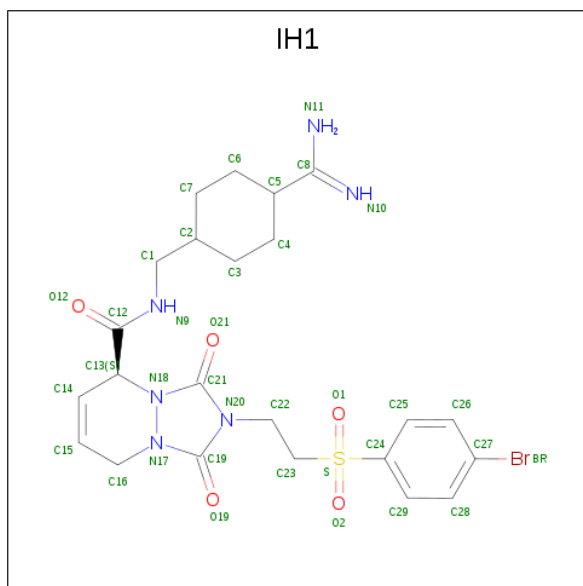
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	554	ALA	-	INSERTION	UNP P28504
3	555	CYS	-	INSERTION	UNP P28504
3	556	GLU	-	INSERTION	UNP P28504
3	557	ASN	-	INSERTION	UNP P28504
3	558	GLU	-	INSERTION	UNP P28504
3	562	GLY	GLU	CONFLICT	UNP P28504
3	565	GLY	GLU	CONFLICT	UNP P28504

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	2	1	Total	Na	0	0
			1	1		

- Molecule 5 is 2-[2-(4-BROMO-BENZENESULFONYL)-ETHYL]-1-3-DIOXO-2,3,5,8-TETRAHYDRO-1H-[1,2,4]TRIAZOLO[1,2-A]PYRIDAZINE-5-CARBOXYLIC ACID(4-CARBAMIMIDOYL-CYCLOHEXYLMETHYL)-AMIDE (three-letter code: IH1) (formula: $C_{23}H_{29}BrN_6O_5S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	2	1	Total	Br	C	N	O	S	0	0
			36	1	23	6	5	1		

- Molecule 6 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	8	Total	O	0	0
			8	8		
6	2	85	Total	O	0	0
			85	85		
6	3	2	Total	O	0	0
			2	2		

3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

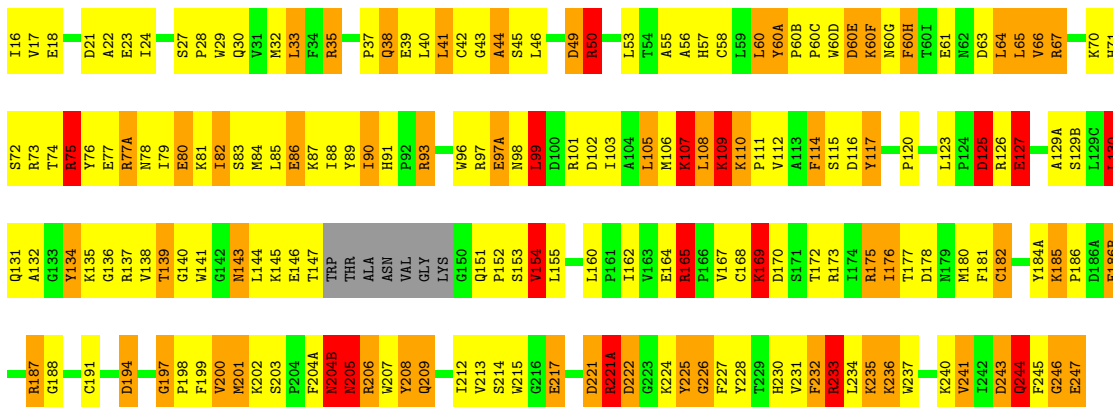
• Molecule 1: thrombin

Chain 1: 



• Molecule 2: thrombin

Chain 2: 



• Molecule 3: PROTEIN (HIRUGEN)

Chain 3: 



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	71.51Å 72.02Å 72.91Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	7.00 – 2.10	Depositor
% Data completeness (in resolution range)	75.0 (7.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.12	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2479	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: NA, IH1, 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	1	1.18	0/242	2.66	17/322 (5.3%)
2	2	1.18	2/2091 (0.1%)	2.70	143/2823 (5.1%)
3	3	1.09	0/53	1.90	1/70 (1.4%)
All	All	1.18	2/2386 (0.1%)	2.68	161/3215 (5.0%)

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	2	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	186(B)	GLU	CD-OE2	-5.80	1.19	1.25
2	2	136	GLY	CA-C	5.79	1.61	1.51

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	187	ARG	NE-CZ-NH1	29.81	135.21	120.30
2	2	126	ARG	NE-CZ-NH1	21.82	131.21	120.30
2	2	221(A)	ARG	NE-CZ-NH2	21.30	130.95	120.30
2	2	126	ARG	CD-NE-CZ	21.24	153.33	123.60
2	2	221(A)	ARG	NE-CZ-NH1	-17.55	111.53	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	165	ARG	Sidechain
2	2	197	GLY	Mainchain
2	2	233	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	1	240	0	239	46	0
2	2	2039	0	2010	238	0
3	3	68	0	52	8	0
4	2	1	0	0	0	0
5	2	36	0	26	5	0
6	1	8	0	0	2	0
6	2	85	0	0	24	0
6	3	2	0	0	0	0
All	All	2479	0	2327	257	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 55.

The worst 5 of 257 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)
2:2:86:GLU:CG	2:2:109:LYS:HZ2	1.22	1.52
2:2:86:GLU:HG3	2:2:109:LYS:NZ	1.16	1.47
1:1:14(K):ILE:CG2	2:2:134:TYR:OH	1.73	1.36
1:1:14(K):ILE:HG22	2:2:134:TYR:CZ	1.62	1.34
1:1:14(K):ILE:HG22	2:2:134:TYR:CE1	1.70	1.26

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	1	28/36 (78%)	23 (82%)	2 (7%)	3 (11%)	0	0
2	2	248/259 (96%)	232 (94%)	14 (6%)	2 (1%)	21	16
3	3	6/14 (43%)	6 (100%)	0	0	100	100
All	All	282/309 (91%)	261 (93%)	16 (6%)	5 (2%)	9	4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	1(C)	GLU
1	1	1(D)	GLY
1	1	1(B)	ALA
2	2	38	GLN
2	2	77(A)	ARG

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	1	27/31 (87%)	23 (85%)	4 (15%)	3	1
2	2	220/225 (98%)	189 (86%)	31 (14%)	4	2
3	3	5/10 (50%)	4 (80%)	1 (20%)	1	0
All	All	252/266 (95%)	216 (86%)	36 (14%)	3	2

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	107	LYS
2	2	127	GLU
2	2	244	GLN
2	2	110	LYS
2	2	129(B)	SER

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

Mol	Chain	Res	Type
2	2	30	GLN
2	2	78	ASN
2	2	156	GLN
2	2	204(B)	ASN
2	2	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	3	567	3	15,16,17	1.48	2 (13%)	19,22,24	1.71	4 (21%)

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	3	567	3	-	0/9/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	567	TYS	OH-CZ	-3.51	1.37	1.42
3	3	567	TYS	CA-C	3.84	1.55	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	567	TYS	OH-S-O2	-4.19	95.49	107.50
3	3	567	TYS	CD1-CE1-CZ	-3.11	115.91	119.73
3	3	567	TYS	O-C-CA	-2.40	118.38	124.96
3	3	567	TYS	O2-S-O1	2.16	121.59	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	3	567	TYS	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	IH1	2	370	-	33,39,39	4.21	19 (57%)	36,57,57	4.07	25 (69%)

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	IH1	2	370	-	-	0/21/45/45	0/3/4/4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	370	IH1	C1-N9	-11.69	1.13	1.46
5	2	370	IH1	C7-C6	-6.55	1.36	1.52
5	2	370	IH1	BR-C27	-6.32	1.77	1.90
5	2	370	IH1	C1-C2	-5.14	1.42	1.51
5	2	370	IH1	C5-C8	-4.80	1.40	1.49

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	370	IH1	O12-C12-N9	-9.08	105.62	123.05
5	2	370	IH1	C6-C5-C8	-6.09	103.46	111.47
5	2	370	IH1	C25-C24-S	-5.83	112.81	119.49
5	2	370	IH1	C4-C5-C8	-5.78	103.87	111.47
5	2	370	IH1	C6-C5-C4	-5.09	98.84	109.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	2	370	IH1	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.