W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2014 – 12:32 AM 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)

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Clashscore		55
Ramachandran outliers		1.8%
Sidechain outliers		14.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
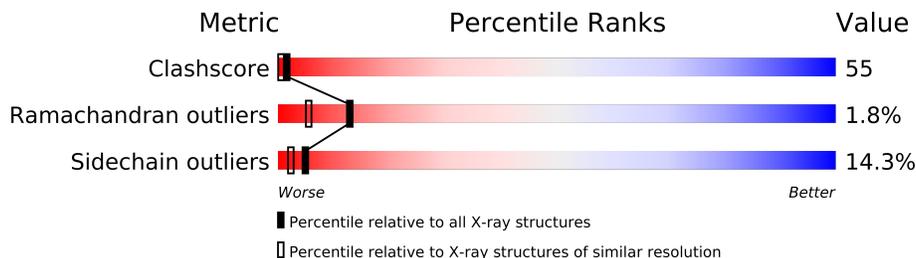
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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 240	C 150	N 39	O 50	S 1	0	0	0

- Molecule 2 is a protein called thrombin.

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

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

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

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 1	Na 1	0	0

- 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-CARBOXYLICACID(4-CARBAMIMIDOYL-CYCLOHEXYLMETHYL)-AMIDE (three-letter code: IH1) (formula: $C_{23}H_{29}BrN_6O_5S$).
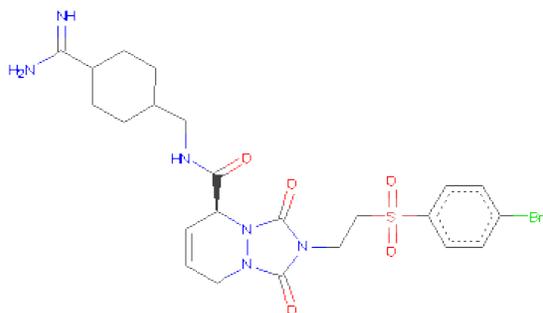
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	S		
5	2	1	36	1	23	6	5	1	0	0

- Molecule 6 is water.

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

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 errors 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:
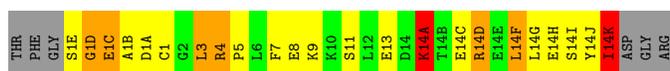
- Molecule 2: thrombin

Chain 2:
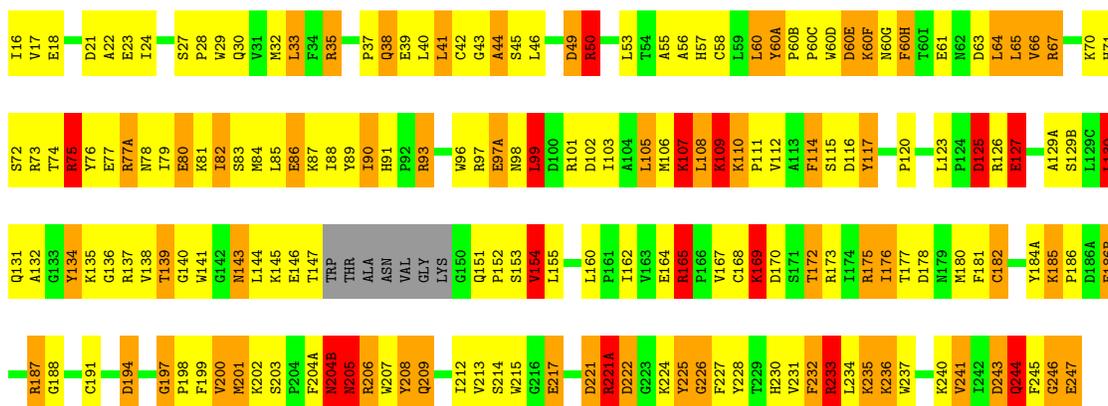
- Molecule 3: PROTEIN (HIRUGEN)

Chain 3:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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(^{o})	Ideal(^{o})
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	240	0	239	46	0
2	2	2039	0	2010	238	1
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	1
6	2	85	0	0	24	2
6	3	2	0	0	0	0
All	All	2479	0	2327	257	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 55.

The worst 5 of 257 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	Distance(Å)	Clash(Å)
6:1:505:HOH:O	6:2:504:HOH:O[3_455]	1.87	0.33
2:2:172:THR:O	6:2:419:HOH:O[4_546]	2.06	0.14

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	1	28/36 (78%)	23 (82%)	2 (7%)	3 (11%)	1	0
2	2	248/259 (96%)	232 (94%)	14 (6%)	2 (1%)	27	20
3	3	6/14 (43%)	6 (100%)	0	0	100	100
All	All	282/309 (91%)	261 (93%)	16 (6%)	5 (2%)	13	5

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 ⓘ

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

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

Mol	Chain	Res	Type
2	2	107	LYS

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Mol	Chain	Res	Type
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 chains 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	16,16,17	5.18	3 (18%)	20,22,24	2.04	5 (25%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	567	TYS	O-C	19.72	1.25	1.11
3	3	567	TYS	OH-CZ	-4.59	1.37	1.42
3	3	567	TYS	CA-C	3.68	1.55	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	567	TYS	C-CA-N	-5.72	108.11	113.83
3	3	567	TYS	OH-S-O2	-4.21	95.49	107.64
3	3	567	TYS	CD1-CE1-CZ	-2.88	115.91	119.76
3	3	567	TYS	CZ-OH-S	2.15	122.21	118.98
3	3	567	TYS	O2-S-O1	2.12	121.59	112.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates 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	IH1	2	370	-	39,39,39	4.80	22 (56%)	46,57,57	4.21	28 (60%)

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	-	-	0/22/45/45	0/2/4/4

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	370	IH1	C13-C12	15.10	1.69	1.53
5	2	370	IH1	C16-N17	-11.37	1.35	1.46
5	2	370	IH1	C13-C14	-10.97	1.41	1.50
5	2	370	IH1	C1-N9	-10.88	1.13	1.46
5	2	370	IH1	C7-C6	-6.47	1.36	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	2	370	IH1	C13-C12-N9	9.78	130.01	115.83
5	2	370	IH1	O12-C12-N9	-8.58	105.62	123.05
5	2	370	IH1	C1-N9-C12	8.58	138.91	122.58
5	2	370	IH1	C7-C6-C5	8.10	124.45	110.81
5	2	370	IH1	C16-N17-N18	7.50	125.50	119.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.