



Full wwPDB X-ray Structure Validation Report i

Feb 26, 2014 – 07:20 PM GMT

PDB ID : 4DJX
Title : Structure of BACE Bound to 5-(3-(5-chloropyridin-3-yl)phenyl)-5-cyclopropyl-2-imino-3-methylimidazolidin-4-one
Authors : Strickland, C.; Cumming, J.
Deposited on : 2012-02-02
Resolution : 1.50 Å (reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

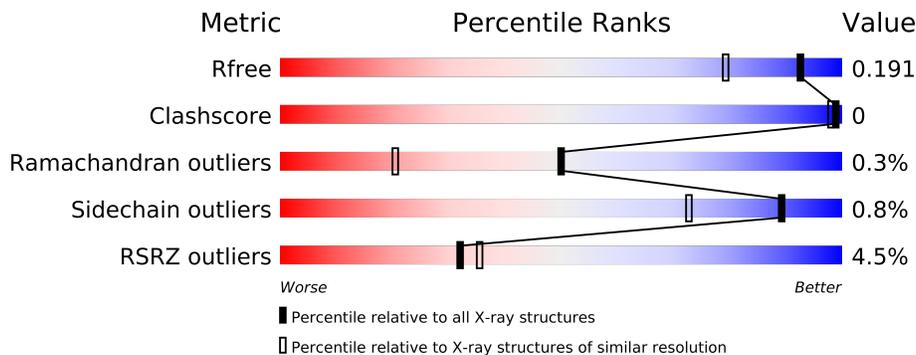
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.50 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))
R_{free}	66092	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

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.

Mol	Chain	Length	Quality of chain
1	A	414	
1	B	414	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	TLA	A	502	-	X
3	TLA	B	502	-	X

2 Entry composition (i)

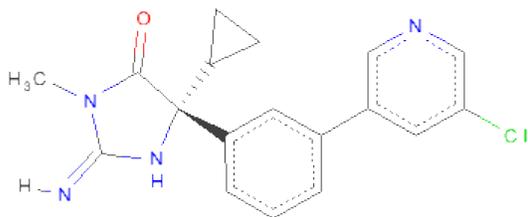
There are 4 unique types of molecules in this entry. The entry contains 7115 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Beta-secretase 1.

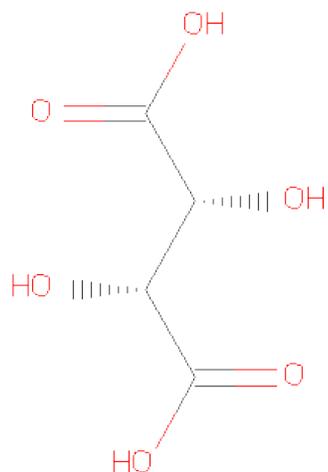
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	Total 3060	C 1959	N 508	O 579	S 14	0	0	0
1	B	389	Total 3052	C 1953	N 507	O 578	S 14	0	0	0

- Molecule 2 is (2E,5R)-5-[3-(5-CHLOROPYRIDIN-3-YL)PHENYL]-5-CYCLOPROPYL-2-IMINO-3-METHYLIMIDAZOLIDIN-4-ONE (three-letter code: 0KQ) (formula: C₁₈H₁₇ClN₄O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	Total 24	C 18	Cl 1	N 4	O 1	0	0
2	B	1	Total 24	C 18	Cl 1	N 4	O 1	0	0

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			10	4 6		
3	B	1	Total	C O	0	0
			10	4 6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	490	Total	O	0	0
			490	490		
4	B	445	Total	O	0	0
			445	445		

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.47Å 89.46Å 131.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 1.50 19.91 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (19.91-1.50) 97.1 (19.91-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.65 (at 1.50Å)	Xtrriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.186 , 0.201 0.177 , 0.191	Depositor DCC
R_{free} test set	7925 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	14.5	Xtrriage
Anisotropy	0.441	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.1	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	0 of 158124 reflections	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7115	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.72 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6927e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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: TLA, 0KQ

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	0.49	0/3138	0.65	0/4267
1	B	0.48	0/3130	0.65	0/4256
All	All	0.49	0/6268	0.65	0/8523

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	A	3060	0	0	2	0
1	B	3052	0	0	0	0
2	A	24	0	15	0	0
2	B	24	0	16	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
4	A	490	0	0	1	0
4	B	445	0	0	0	0
All	All	7115	0	39	2	0

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 0.

All (2) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:279:LYS:CE	4:A:863:HOH:O	2.62	0.48
1:A:186:GLU:OE1	1:A:256:ARG:NH1	2.53	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

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	388/414 (94%)	378 (97%)	9 (2%)	1 (0%)	50	20
1	B	387/414 (94%)	377 (97%)	9 (2%)	1 (0%)	50	20
All	All	775/828 (94%)	755 (97%)	18 (2%)	2 (0%)	50	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	SER
1	B	376	SER

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	332/355 (94%)	330 (99%)	2 (1%)	92	80
1	B	331/355 (93%)	328 (99%)	3 (1%)	87	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	663/710 (93%)	658 (99%)	5 (1%)	89	73

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	258	TRP
1	B	134	GLN
1	B	172	ASN
1	B	258	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are 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	OKQ	A	501	-	27,27,27	1.01	3 (11%)	41,41,41	1.18	5 (12%)
3	TLA	A	502	-	9,9,9	0.27	0	12,12,12	0.35	0
2	OKQ	B	501	-	27,27,27	1.16	2 (7%)	41,41,41	1.30	7 (17%)
3	TLA	B	502	-	9,9,9	0.19	0	12,12,12	0.35	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
2	OKQ	A	501	-	-	0/16/37/37	0/3/4/4
3	TLA	A	502	-	-	0/12/12/12	0/0/0/0
2	OKQ	B	501	-	-	0/16/37/37	0/3/4/4
3	TLA	B	502	-	-	0/12/12/12	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	OKQ	C2-N1	4.41	1.52	1.46
2	A	501	OKQ	C2-N1	3.43	1.50	1.46
2	B	501	OKQ	C3-N2	3.25	1.42	1.38
2	A	501	OKQ	C3-N1	2.75	1.36	1.34
2	A	501	OKQ	C3-N2	2.34	1.41	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	OKQ	C6-C2-C1	-4.60	104.14	111.19
2	A	501	OKQ	C6-C2-C1	-3.86	105.27	111.19
2	A	501	OKQ	C5-C2-C6	3.35	117.30	111.80
2	B	501	OKQ	C4-N2-C3	2.65	126.59	124.71
2	B	501	OKQ	C5-C2-C6	2.59	116.05	111.80
2	A	501	OKQ	N1-C3-N2	2.51	112.08	108.39
2	A	501	OKQ	C4-N2-C3	2.43	126.43	124.71
2	B	501	OKQ	N1-C3-N2	2.42	111.95	108.39
2	B	501	OKQ	C5-C2-N1	-2.35	107.91	111.42
2	A	501	OKQ	C2-N1-C3	-2.11	108.01	112.28
2	B	501	OKQ	C6-C2-N1	2.08	115.02	110.99
2	B	501	OKQ	C2-N1-C3	-2.05	108.14	112.28

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	390/414 (94%)	0.06	19 (4%) 28 32	9, 16, 36, 68	0
1	B	389/414 (93%)	0.02	16 (4%) 35 39	10, 16, 33, 63	0
All	All	779/828 (94%)	0.04	35 (4%) 32 35	9, 16, 35, 68	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	VAL	11.0
1	A	375	THR	10.5
1	B	373	VAL	10.3
1	B	375	THR	10.1
1	A	447	ILE	8.4
1	B	133	THR	8.2
1	A	134	GLN	6.2
1	B	134	GLN	5.7
1	B	441	GLU	4.7
1	B	374	ALA	4.7
1	B	224	GLN	4.5
1	A	374	ALA	4.3
1	A	224	GLN	3.8
1	A	132	TYR	3.6
1	A	58	GLY	3.3
1	A	376	SER	3.2
1	B	132	TYR	3.1
1	A	133	THR	3.0
1	A	441	GLU	3.0
1	B	438	LEU	3.0
1	B	59	SER	2.8
1	A	59	SER	2.8
1	B	206	HIS	2.7
1	A	129	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	172	ASN	2.6
1	A	206	HIS	2.6
1	B	326	GLU	2.3
1	A	438	LEU	2.3
1	A	108	PHE	2.2
1	B	105	PRO	2.2
1	B	445	TYR	2.1
1	A	110	HIS	2.1
1	B	135	GLY	2.1
1	A	107	PRO	2.1
1	B	58	GLY	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q < 0.9
3	TLA	A	502	10/10	0.34	5.50	26,36,39,40	0
3	TLA	B	502	10/10	0.25	5.31	25,31,35,36	0
2	0KQ	B	501	24/24	0.06	-0.13	12,14,17,21	0
2	0KQ	A	501	24/24	0.06	-0.31	11,14,17,18	0

6.5 Other polymers (i)

There are no such residues in this entry.