



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:51 am GMT

PDB ID : 5HU0
Title : BACE1 in complex with 4-(3-(furan-2-carboxamido)phenyl)-1-methyl-5-oxo-4-phenylimidazolidin-2-iminium
Authors : Orth, P.
Deposited on : 2016-01-27
Resolution : 1.83 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

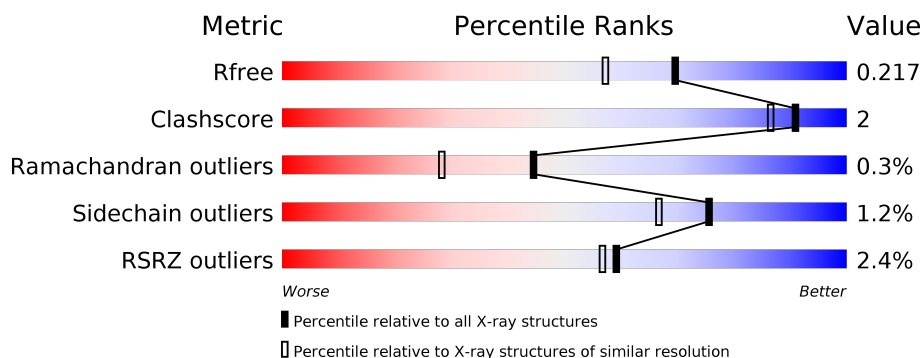
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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}	100719	2964 (1.86-1.82)
Clashscore	112137	3197 (1.86-1.82)
Ramachandran outliers	110173	3164 (1.86-1.82)
Sidechain outliers	110143	3165 (1.86-1.82)
RSRZ outliers	101464	2973 (1.86-1.82)

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.

Mol	Chain	Length	Quality of chain
1	A	412	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>5%</div> </div> </div>
1	B	412	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>6%</div> </div> </div>

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
2	TLA	A	501	-	-	-	X
2	TLA	B	501	-	-	-	X

2 Entry composition [i](#)

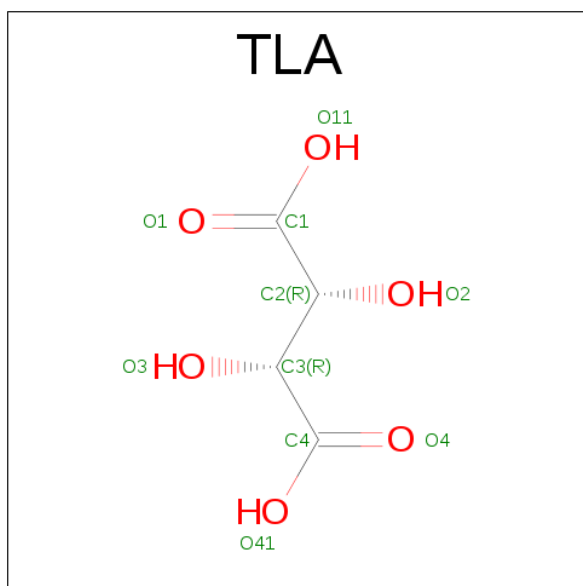
There are 4 unique types of molecules in this entry. The entry contains 7109 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-secretase 1.

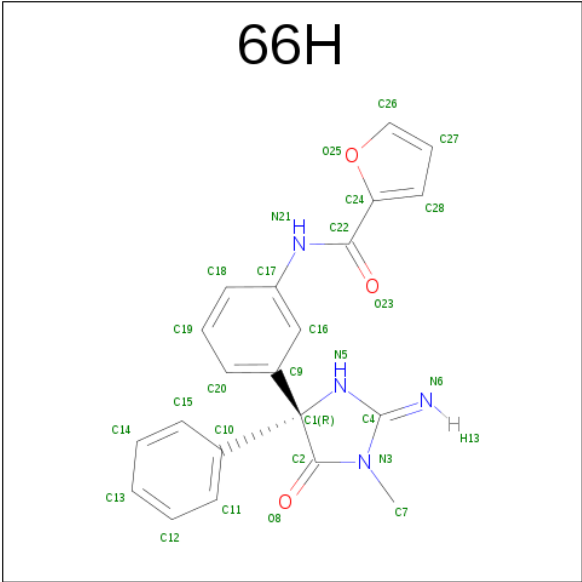
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3056	1956	507	579	14			
1	B	389	Total	C	N	O	S	0	0	0
			3052	1953	507	578	14			

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



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

- Molecule 3 is N-{3-[(2E,4R)-2-imino-1-methyl-5-oxo-4-phenylimidazolidin-4-yl]phenyl}furan-2-carboxamide (three-letter code: 66H) (formula: C₂₁H₁₈N₄O₃).

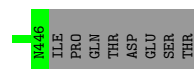


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	21	4	3		
3	B	1	Total	C	N	O	0	0
			28	21	4	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	466	Total	O	0	0
			466	466		
4	B	459	Total	O	0	0
			459	459		

- Molecule 1: Beta-secretase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.47Å 89.82Å 131.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 1.83 19.93 – 1.83	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.97-1.83) 98.3 (19.93-1.83)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.82Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.169 , 0.199 0.182 , 0.217	Depositor DCC
R_{free} test set	3589 reflections (4.21%)	DCC
Wilson B-factor (Å ²)	12.3	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7109	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.40 % 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 1.1511e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TLA, 66H

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	0.51	0/3134	0.65	0/4263
1	B	0.51	0/3130	0.66	0/4256
All	All	0.51	0/6264	0.65	0/8519

There are no bond length outliers.

There are no bond angle outliers.

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	A	3056	0	2959	14	0
1	B	3052	0	2959	10	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
4	A	466	0	0	2	0
4	B	459	0	0	1	0
All	All	7109	0	5926	24	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 2.

All (24) 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:A:361:ILE:HD13	1:A:398:ILE:HD12	1.65	0.77
1:A:125:ARG:HD3	4:A:823:HOH:O	1.99	0.63
1:A:361:ILE:HD13	1:A:398:ILE:CD1	2.33	0.57
1:A:63:MET:HG2	1:A:151:GLY:HA2	1.87	0.56
1:B:132:TYR:HE2	1:B:134:GLN:HG2	1.73	0.54
1:A:58:GLY:HA2	1:A:242:HIS:HD2	1.73	0.53
1:B:132:TYR:CE2	1:B:134:GLN:HG2	2.44	0.53
1:A:333:ALA:HB2	1:A:377:GLN:O	2.09	0.52
1:B:333:ALA:HB2	1:B:377:GLN:O	2.10	0.51
1:B:134:GLN:HG3	4:B:774:HOH:O	2.09	0.50
1:A:171:ILE:HB	1:A:174:SER:HB3	1.93	0.50
1:A:423:HIS:HD2	1:A:424:ASP:O	1.95	0.50
1:B:423:HIS:HD2	1:B:424:ASP:O	1.95	0.49
1:B:171:ILE:HB	1:B:174:SER:HB3	1.96	0.47
1:A:156:VAL:HG11	1:A:201:LEU:HA	1.96	0.46
1:A:295:LEU:HB2	1:A:398:ILE:HD11	2.00	0.42
1:A:439:ASP:O	1:A:442:ASP:HB2	2.19	0.42
1:A:266:ARG:HB3	1:A:347:TYR:HB2	2.02	0.42
1:B:439:ASP:O	1:B:442:ASP:HB2	2.19	0.42
1:B:295:LEU:HB2	1:B:398:ILE:HD11	2.03	0.41
1:B:266:ARG:HB3	1:B:347:TYR:HB2	2.02	0.41
1:A:58:GLY:HA2	1:A:242:HIS:CD2	2.55	0.40
1:B:62:GLU:HG2	1:B:63:MET:HG3	2.04	0.40
1:A:62:GLU:HB2	4:A:916:HOH:O	2.20	0.40

There are no symmetry-related clashes.

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	A	388/412 (94%)	381 (98%)	6 (2%)	1 (0%)	44	28
1	B	387/412 (94%)	381 (98%)	5 (1%)	1 (0%)	44	28
All	All	775/824 (94%)	762 (98%)	11 (1%)	2 (0%)	44	28

All (2) Ramachandran outliers are listed below:

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

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	A	331/353 (94%)	327 (99%)	4 (1%)	75	67
1	B	331/353 (94%)	327 (99%)	4 (1%)	75	67
All	All	662/706 (94%)	654 (99%)	8 (1%)	75	67

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	SER
1	A	258	TRP
1	A	328	LEU
1	A	375	THR
1	B	225	SER
1	B	258	TRP
1	B	328	LEU
1	B	375	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN

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Mol	Chain	Res	Type
1	A	423	HIS
1	A	446	ASN
1	B	89	ASN
1	B	172	ASN
1	B	423	HIS

5.3.3 RNA [i](#)

There are no RNA molecules 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	TLA	A	501	-	3,9,9	0.23	0	6,12,12	0.67	0
3	66H	A	502	-	28,31,31	1.08	3 (10%)	35,45,45	1.13	4 (11%)
2	TLA	B	501	-	3,9,9	0.27	0	6,12,12	0.79	0
3	66H	B	502	-	28,31,31	1.10	4 (14%)	35,45,45	1.19	4 (11%)

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	TLA	A	501	-	-	0/4/12/12	0/0/0/0
3	66H	A	502	-	-	0/17/39/39	0/3/4/4
2	TLA	B	501	-	-	0/4/12/12	0/0/0/0
3	66H	B	502	-	-	0/17/39/39	0/3/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	66H	C24-C22	-3.49	1.44	1.49
3	A	502	66H	C24-C22	-3.15	1.44	1.49
3	A	502	66H	C4-N6	-2.78	1.29	1.33
3	B	502	66H	C1-C2	-2.31	1.51	1.55
3	A	502	66H	C1-C2	-2.13	1.51	1.55
3	B	502	66H	C4-N6	-2.07	1.30	1.33
3	B	502	66H	C1-C9	-2.07	1.50	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	66H	C10-C1-N5	-2.70	107.75	111.56
3	A	502	66H	C9-C1-C2	-2.02	105.75	110.41
3	B	502	66H	C17-C16-C9	2.04	122.27	119.81
3	A	502	66H	C10-C1-C9	2.08	116.14	112.60
3	A	502	66H	C17-C16-C9	2.14	122.39	119.81
3	B	502	66H	C10-C1-C9	2.17	116.28	112.60
3	A	502	66H	C2-C1-N5	2.67	101.21	99.21
3	B	502	66H	C1-N5-C4	2.81	112.92	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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	390/412 (94%)	-0.38	10 (2%) 56 53	6, 13, 35, 77	0
1	B	389/412 (94%)	-0.39	9 (2%) 61 58	7, 13, 33, 61	0
All	All	779/824 (94%)	-0.39	19 (2%) 59 57	6, 13, 33, 77	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	VAL	9.6
1	B	375	THR	9.5
1	A	375	THR	8.4
1	B	373	VAL	8.1
1	B	59	SER	4.4
1	B	441	GLU	4.3
1	A	447	ILE	3.7
1	B	374	ALA	3.7
1	A	374	ALA	3.2
1	A	171	ILE	3.1
1	B	133	THR	3.1
1	A	441	GLU	3.1
1	A	110	HIS	2.7
1	B	58	GLY	2.7
1	A	133	THR	2.6
1	B	206	HIS	2.4
1	A	206	HIS	2.1
1	B	134	GLN	2.1
1	A	129	TYR	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	TLA	B	501	10/10	0.91	0.27	6.35	33,37,39,39	0
2	TLA	A	501	10/10	0.66	0.38	4.54	48,51,53,54	0
3	66H	A	502	28/28	0.97	0.07	-0.40	9,12,17,19	0
3	66H	B	502	28/28	0.98	0.07	-0.41	6,10,14,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.