



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:30 PM GMT

PDB ID : 3INE  
Title : Bace1 with the aminohydantoin Compound S-34  
Authors : Olland, A.M.; Chopra, R.  
Deposited on : 2009-08-12  
Resolution : 2.00 Å(reported)

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

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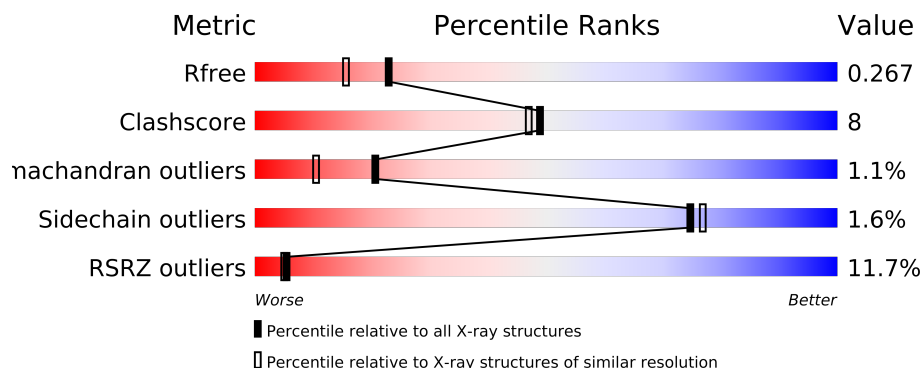
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	415	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3030 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.

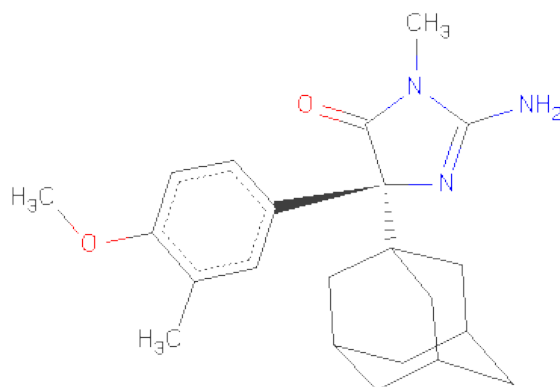
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	367	2881	1850	481	536	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	HIS	-	expression tag	UNP P56817
A	457	HIS	-	expression tag	UNP P56817
A	458	HIS	-	expression tag	UNP P56817
A	459	HIS	-	expression tag	UNP P56817
A	460	HIS	-	expression tag	UNP P56817
A	461	HIS	-	expression tag	UNP P56817

- Molecule 2 is (5S)-2-AMINO-5-(4-METHOXY-3-METHYLPHENYL)-3-METHYL-5-[(3S,5S,7S)-TRICYCLO[3.3.1.1<sup>3,7</sup>]DEC-1-YL]-3,5-DIHYDRO-4H-IMIDAZOL-4-ONE (three-letter code: X17) (formula: C<sub>22</sub>H<sub>29</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	22	3	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.14Å 104.33Å 49.55Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00 20.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.7 ((Not available)-2.00) 91.8 (20.06-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.219 , 0.276 0.214 , 0.267	Depositor DCC
$R_{free}$ test set	1166 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.987	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 36.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 23099 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: X17

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	0.30	0/2953	0.49	0/4008

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

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	2881	0	2794	44	0
2	A	27	0	29	0	0
3	A	122	0	0	4	0
All	All	3030	0	2823	44	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 8.

All (44) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:130:TYR:CE2	1:A:132:PRO:HG3	2.07	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:296:LEU:HB2	1:A:399:ILE:HD11	1.68	0.74
1:A:316:THR:O	1:A:317:GLU:HB2	1.92	0.68
1:A:428:ARG:HD2	3:A:43:HOH:O	2.00	0.62
1:A:314:SER:HA	1:A:341:ILE:HG22	1.84	0.59
1:A:284:TYR:HD1	1:A:446:TYR:CZ	2.23	0.57
1:A:137:LYS:HE2	1:A:139:GLU:OE2	2.08	0.54
1:A:356:GLN:NE2	1:A:435:PRO:HB3	2.23	0.53
1:A:315:SER:O	1:A:317:GLU:N	2.41	0.53
1:A:284:TYR:CD1	1:A:446:TYR:CZ	2.96	0.53
1:A:338:PRO:HB2	1:A:341:ILE:HG13	1.91	0.52
1:A:424:HIS:CD2	1:A:429:THR:HG22	2.44	0.52
1:A:284:TYR:HD1	1:A:446:TYR:CE1	2.28	0.52
1:A:446:TYR:O	1:A:447:ASN:C	2.48	0.51
1:A:111:HIS:HB3	3:A:533:HOH:O	2.11	0.49
1:A:133:TYR:CE2	1:A:137:LYS:HA	2.47	0.49
1:A:381:CYS:N	3:A:4:HOH:O	2.45	0.49
1:A:316:THR:O	1:A:317:GLU:CB	2.58	0.47
1:A:89:LEU:HD13	1:A:102:VAL:HG11	1.97	0.47
1:A:204:LYS:HE3	3:A:505:HOH:O	2.14	0.46
1:A:284:TYR:CD1	1:A:446:TYR:CE1	3.04	0.46
1:A:127:LYS:HD2	1:A:142:LEU:HD12	1.96	0.46
1:A:132:PRO:HA	1:A:137:LYS:HB2	1.98	0.46
1:A:104:ALA:CB	1:A:163:ALA:HB1	2.46	0.46
1:A:187:GLU:OE2	1:A:257:ARG:NH2	2.45	0.45
1:A:266:VAL:HG21	1:A:438:THR:HG21	1.99	0.45
1:A:315:SER:O	1:A:318:LYS:HD2	2.17	0.45
1:A:157:VAL:HG11	1:A:202:LEU:HA	1.99	0.45
1:A:130:TYR:HD1	1:A:139:GLU:HB3	1.83	0.44
1:A:261:TYR:HB3	1:A:414:ILE:HD11	2.00	0.44
1:A:353:VAL:O	1:A:354:THR:C	2.57	0.43
1:A:317:GLU:HG2	1:A:319:PHE:CZ	2.54	0.43
1:A:216:LEU:O	1:A:401:GLU:HA	2.19	0.43
1:A:297:ARG:HB3	1:A:389:SER:HB2	2.00	0.42
1:A:284:TYR:HA	1:A:285:ASP:HA	1.62	0.42
1:A:329:LEU:HD12	1:A:329:LEU:O	2.19	0.42
1:A:264:ILE:HB	1:A:350:MET:HE3	2.02	0.42
1:A:113:TYR:CE1	1:A:115:GLN:HG2	2.55	0.41
1:A:130:TYR:CZ	1:A:132:PRO:HG3	2.53	0.41
1:A:66:ASP:CG	1:A:69:ARG:HH12	2.23	0.41
1:A:259:TRP:CG	1:A:260:TYR:N	2.89	0.41
1:A:267:ARG:HG2	1:A:268:VAL:N	2.36	0.41
1:A:366:GLN:O	1:A:398:VAL:HB	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:ASN:OD1	1:A:68:LEU:HD13	2.21	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	357/415 (86%)	341 (96%)	12 (3%)	4 (1%)	21 10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	GLU
1	A	354	THR
1	A	316	THR
1	A	334	ALA

### 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	309/356 (87%)	304 (98%)	5 (2%)	75 77

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

Mol	Chain	Res	Type
1	A	126	ARG
1	A	259	TRP
1	A	268	VAL

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Mol	Chain	Res	Type
1	A	347	LEU
1	A	428	ARG

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand 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	$\# Z  > 2$
2	X17	A	1	-	31,31,31	0.89	1 (3%)	50,50,50	0.72	2 (4%)

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	X17	A	1	-	-	0/11/63/63	0/2/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	X17	C9-N2	2.75	1.50	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	X17	C10-C9-N2	-2.62	101.13	103.83
2	A	1	X17	N3-C11-N1	-2.06	121.16	122.72

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	367/415 (88%)	0.62	43 (11%) 5 5	15, 25, 52, 71	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ALA	9.1
1	A	423	VAL	8.4
1	A	354	THR	8.3
1	A	424	HIS	8.0
1	A	427	PHE	5.8
1	A	221	PHE	5.8
1	A	220	GLY	5.0
1	A	60	SER	4.7
1	A	327	GLU	4.5
1	A	381	CYS	3.9
1	A	341	ILE	3.7
1	A	426	GLU	3.5
1	A	447	ASN	3.4
1	A	422	HIS	3.4
1	A	333	GLN	3.3
1	A	126	ARG	3.2
1	A	325	LEU	3.1
1	A	446	TYR	3.1
1	A	355	ASN	3.0
1	A	329	LEU	3.0
1	A	62	VAL	3.0
1	A	441	MET	2.9
1	A	133	TYR	2.9
1	A	328	GLN	2.8
1	A	316	THR	2.8
1	A	335	GLY	2.8
1	A	438	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	284	TYR	2.7
1	A	300	LYS	2.6
1	A	130	TYR	2.6
1	A	353	VAL	2.6
1	A	273	GLN	2.5
1	A	442	GLU	2.4
1	A	169	LYS	2.4
1	A	276	LYS	2.4
1	A	134	THR	2.4
1	A	230	ALA	2.2
1	A	111	HIS	2.2
1	A	207	HIS	2.1
1	A	332	TRP	2.1
1	A	164	ILE	2.1
1	A	330	VAL	2.1
1	A	420	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	X17	A	1	27/27	0.09	-0.69	16,21,24,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.