



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 12:28 pm GMT

PDB ID : 1W50  
Title : Apo Structure of BACE (Beta Secretase)  
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Deposited on : 2004-08-04  
Resolution : 1.75 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

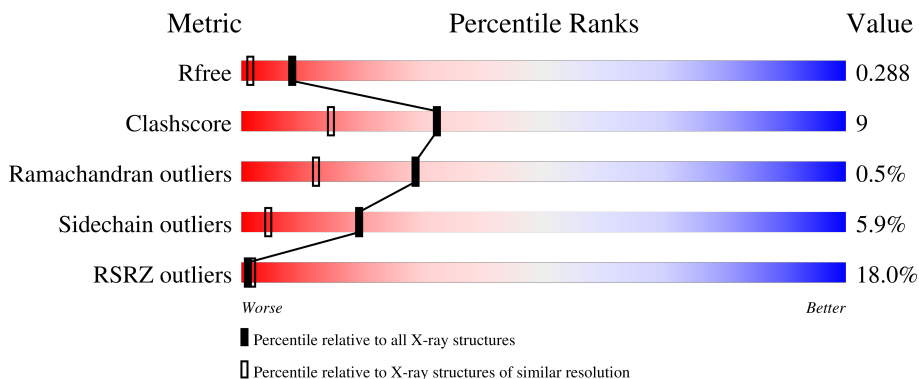
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	411	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3249 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
			Total	C	N	O	S			
1	A	378	2966	1898	494	560	14	26	0	1

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	I	0	0
			4	4		

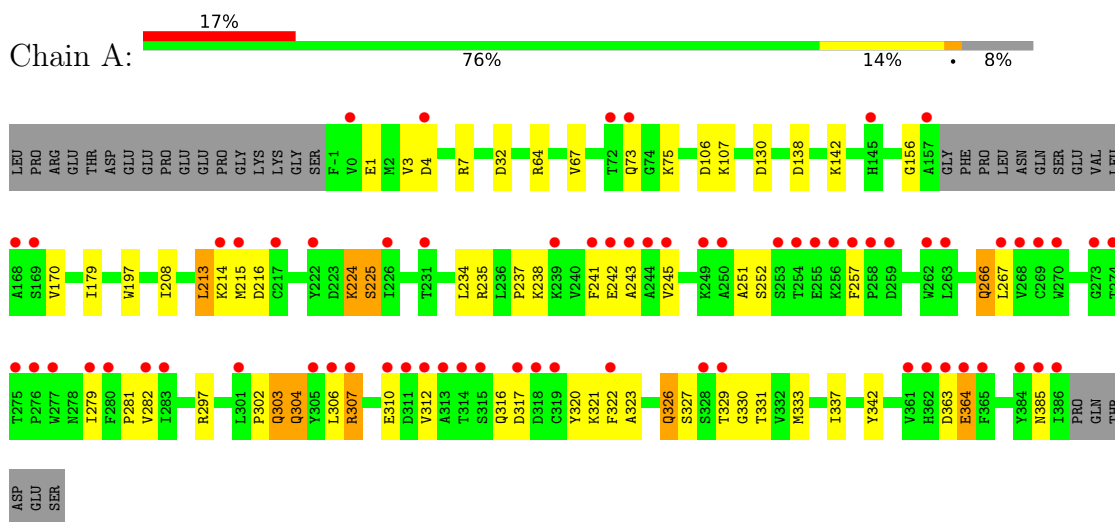
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	279	Total	O	0	0
			279	279		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

- Molecule 1: BETA-SECRETASE 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.24Å 103.24Å 169.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.52 – 1.75 39.52 – 1.75	Depositor EDS
% Data completeness (in resolution range)	95.1 (39.52-1.75) 95.1 (39.52-1.75)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.1.29	Depositor
R, $R_{free}$	0.244 , 0.283 0.248 , 0.288	Depositor DCC
$R_{free}$ test set	2624 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtrriage
Anisotropy	0.143	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.78	5/3041 (0.2%)	0.87	10/4134 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	GLU	CB-CG	-17.66	1.18	1.52
1	A	64	ARG	CD-NE	13.51	1.69	1.46
1	A	7	ARG	CD-NE	-10.21	1.29	1.46
1	A	266	GLN	CB-CG	5.17	1.66	1.52
1	A	142	LYS	CE-NZ	5.15	1.61	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ARG	CD-NE-CZ	-9.43	110.40	123.60
1	A	7	ARG	CD-NE-CZ	8.96	136.14	123.60
1	A	7	ARG	CG-CD-NE	7.76	128.10	111.80
1	A	32	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	138	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	317	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	142	LYS	CD-CE-NZ	-5.80	98.36	111.70
1	A	130	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	106	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	385	ASN	O-C-N	-5.01	114.69	122.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	2966	0	2878	49	0
2	A	4	0	0	2	0
3	A	279	0	0	25	0
All	All	3249	0	2878	51	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 9.

All (51) 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:A:1505:IOD:I	3:A:2088:HOH:O	2.35	1.13
1:A:304:GLN:HE21	1:A:304:GLN:N	1.53	1.06
2:A:1503:IOD:I	3:A:2122:HOH:O	2.51	0.99
1:A:237:PRO:HA	3:A:2253:HOH:O	1.69	0.90
1:A:251:ALA:HB3	3:A:2214:HOH:O	1.74	0.88
1:A:330:GLY:O	3:A:2254:HOH:O	1.95	0.84
1:A:281:PRO:C	3:A:2226:HOH:O	2.18	0.82
1:A:281:PRO:HD3	3:A:2219:HOH:O	1.87	0.73
1:A:242:GLU:HG2	3:A:2251:HOH:O	1.89	0.72
1:A:252:SER:HB3	3:A:2219:HOH:O	1.90	0.69
1:A:303:GLN:C	1:A:304:GLN:HE21	1.94	0.69
1:A:282:VAL:N	3:A:2226:HOH:O	2.29	0.66
1:A:215:MET:CE	1:A:243:ALA:HB3	2.26	0.65
1:A:73:GLN:O	1:A:107:LYS:HD2	1.97	0.65
1:A:326:GLN:NE2	3:A:2251:HOH:O	2.31	0.63
1:A:330:GLY:N	3:A:2198:HOH:O	2.32	0.61
1:A:235:ARG:HB3	1:A:327:SER:OG	2.00	0.60
1:A:224:LYS:NZ	3:A:2200:HOH:O	2.33	0.60
1:A:224:LYS:NZ	1:A:329:THR:O	2.29	0.59
1:A:215:MET:HE1	1:A:243:ALA:HB3	1.86	0.58
1:A:279:ILE:HG23	3:A:2218:HOH:O	2.06	0.56
1:A:208:ILE:HD12	1:A:213:LEU:HD11	1.88	0.55
1:A:225:SER:HB2	3:A:2201:HOH:O	2.06	0.55
1:A:156:GLY:HA2	1:A:170:VAL:HG12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ARG:HD3	1:A:323:ALA:HB2	1.94	0.50
1:A:225:SER:OG	1:A:331:THR:HB	2.11	0.50
1:A:215:MET:HE2	1:A:243:ALA:HB3	1.92	0.50
1:A:303:GLN:C	1:A:304:GLN:NE2	2.63	0.49
1:A:304:GLN:HE21	1:A:304:GLN:CA	2.21	0.49
1:A:215:MET:O	1:A:216:ASP:C	2.51	0.48
1:A:252:SER:N	3:A:2219:HOH:O	2.46	0.48
1:A:333:MET:CE	1:A:337:ILE:HG21	2.43	0.48
1:A:302:PRO:O	1:A:306:LEU:HB2	2.14	0.48
1:A:156:GLY:HA2	1:A:170:VAL:CB	2.44	0.47
1:A:215:MET:HE2	1:A:243:ALA:CB	2.45	0.46
1:A:156:GLY:HA2	1:A:170:VAL:CG1	2.46	0.45
1:A:224:LYS:O	1:A:331:THR:N	2.44	0.45
1:A:333:MET:HE2	1:A:337:ILE:HG21	1.97	0.45
1:A:179:ILE:HG23	1:A:342:TYR:HE2	1.82	0.44
1:A:156:GLY:HA2	1:A:170:VAL:HB	1.99	0.44
1:A:241:PHE:CZ	1:A:245:VAL:HG21	2.53	0.43
1:A:364:GLU:HB3	3:A:2262:HOH:O	2.17	0.43
1:A:303:GLN:OE1	3:A:2240:HOH:O	2.21	0.42
1:A:107:LYS:HA	3:A:2125:HOH:O	2.19	0.42
1:A:329:THR:C	3:A:2198:HOH:O	2.56	0.42
1:A:320:TYR:HB3	3:A:2248:HOH:O	2.19	0.41
1:A:322:PHE:HA	3:A:2249:HOH:O	2.20	0.41
1:A:3:VAL:O	1:A:4:ASP:CG	2.59	0.40
1:A:321:LYS:C	3:A:2248:HOH:O	2.59	0.40
1:A:225:SER:N	3:A:2201:HOH:O	2.53	0.40
1:A:297:ARG:HG3	3:A:2237:HOH:O	2.22	0.40

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	A	374/411 (91%)	355 (95%)	17 (4%)	2 (0%)	29 12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	GLU
1	A	363	ASP

### 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	321/352 (91%)	302 (94%)	19 (6%)	19 4

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	A	75	LYS
1	A	197	TRP
1	A	213	LEU
1	A	214	LYS
1	A	224	LYS
1	A	225	SER
1	A	234	LEU
1	A	238	LYS
1	A	257	PHE
1	A	266	GLN
1	A	267	LEU
1	A	303	GLN
1	A	304	GLN
1	A	307	ARG
1	A	312	VAL
1	A	316	GLN
1	A	326	GLN
1	A	364	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	211	GLN
1	A	304	GLN
1	A	360	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [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

### 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	378/411 (91%)	0.96	68 (17%) <b>1</b> <b>2</b>	15, 30, 64, 94	11 (2%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	ALA	11.7
1	A	157	ALA	11.2
1	A	315	SER	8.3
1	A	312	VAL	7.8
1	A	279	ILE	6.6
1	A	270	TRP	6.3
1	A	314	THR	5.5
1	A	311	ASP	5.5
1	A	319	CYS	5.5
1	A	365	PHE	5.5
1	A	269	CYS	5.4
1	A	168	ALA	5.3
1	A	273	GLY	5.2
1	A	259	ASP	5.1
1	A	257	PHE	4.9
1	A	0	VAL	4.9
1	A	277	TRP	4.6
1	A	328	SER	4.5
1	A	245	VAL	4.5
1	A	217	CYS	4.4
1	A	276	PRO	4.2
1	A	280	PHE	4.2
1	A	384	TYR	4.2
1	A	222	TYR	4.0
1	A	318	ASP	4.0
1	A	262	TRP	3.9
1	A	250	ALA	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	254	THR	3.7
1	A	256	LYS	3.6
1	A	274	THR	3.6
1	A	307	ARG	3.5
1	A	275	THR	3.5
1	A	267	LEU	3.4
1	A	214	LYS	3.3
1	A	385	ASN	3.3
1	A	283	ILE	3.2
1	A	73	GLN	3.2
1	A	305	TYR	3.2
1	A	317	ASP	3.2
1	A	364	GLU	3.2
1	A	361	VAL	3.1
1	A	363	ASP	2.9
1	A	322	PHE	2.9
1	A	263	LEU	2.8
1	A	4	ASP	2.8
1	A	255	GLU	2.7
1	A	329	THR	2.6
1	A	253	SER	2.6
1	A	310	GLU	2.5
1	A	282	VAL	2.4
1	A	226	ILE	2.4
1	A	72	THR	2.3
1	A	215	MET	2.3
1	A	268	VAL	2.3
1	A	243	ALA	2.2
1	A	301	LEU	2.2
1	A	249	LYS	2.2
1	A	244	ALA	2.1
1	A	145	HIS	2.1
1	A	258	PRO	2.1
1	A	241	PHE	2.1
1	A	169	SER	2.1
1	A	386	ILE	2.1
1	A	239	LYS	2.0
1	A	231	THR	2.0
1	A	362	HIS	2.0
1	A	242	GLU	2.0
1	A	306	LEU	2.0

## 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 monosaccharides 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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IOD	A	1504	1/1	0.92	0.20	54,54,54,54	1
2	IOD	A	1505	1/1	0.97	0.04	56,56,56,56	1
2	IOD	A	1503	1/1	0.99	0.03	35,35,35,35	1
2	IOD	A	1502	1/1	1.00	0.04	23,23,23,23	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.