



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 10:36 pm BST

PDB ID : 1XN3
Title : Crystal structure of Beta-secretase bound to a long inhibitor with additional upstream residues.
Authors : Turner III, R.T.; Hong, L.; Koelsch, G.; Ghosh, A.K.; Tang, J.
Deposited on : 2004-10-04
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

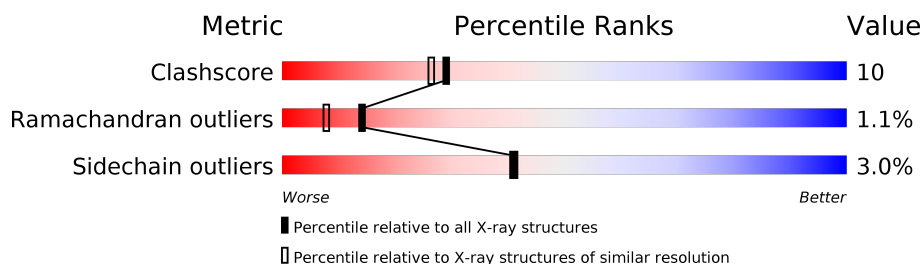
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 ≥ 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	389	
1	B	389	
1	C	389	
1	D	389	
2	I	14	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13072 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	389	Total	C	N	O	S	0	0	0
			3053	1953	507	579	14			
1	B	389	Total	C	N	O	S	0	0	0
			3053	1953	507	579	14			
1	C	389	Total	C	N	O	S	0	0	0
			3053	1953	507	579	14			
1	D	389	Total	C	N	O	S	0	0	0
			3053	1953	507	579	14			

- Molecule 2 is a protein called Peptidic inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	14	Total	C	N	O	0	0	0
			116	73	16	27			

- Molecule 3 is water.

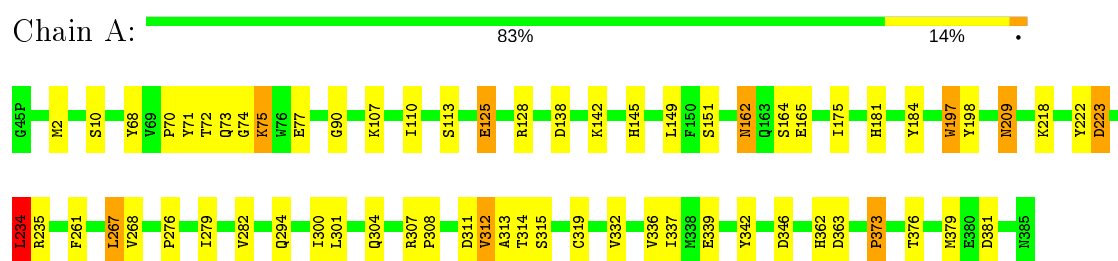
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	196	Total	O	0	0
			196	196		
3	B	184	Total	O	0	0
			184	184		
3	C	190	Total	O	0	0
			190	190		
3	D	167	Total	O	0	0
			167	167		
3	I	7	Total	O	0	0
			7	7		

3 Residue-property plots [i](#)

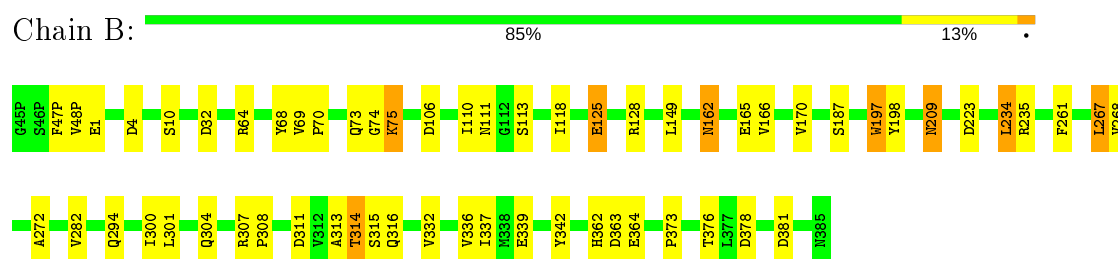
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

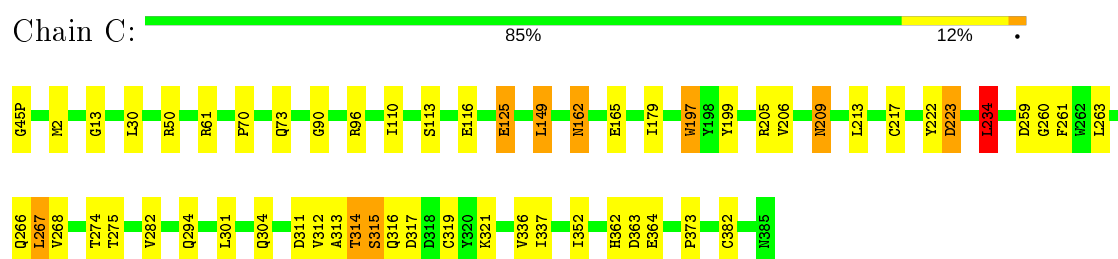
• Molecule 1: Beta-secretase 1



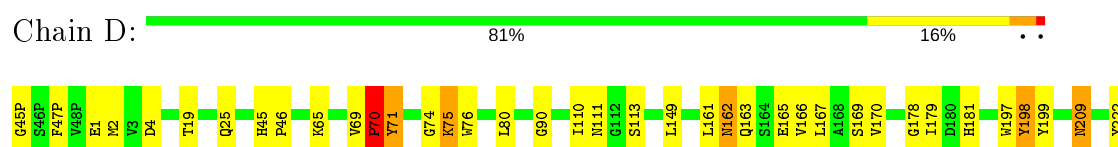
• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1

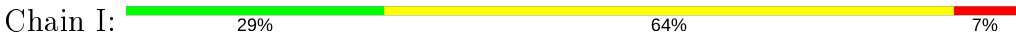


• Molecule 1: Beta-secretase 1





● Molecule 2: Peptidic inhibitor



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.16Å 130.87Å 88.57Å 90.00° 97.27° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.202 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13072	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

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: STA

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	0.50	0/3131	0.74	3/4256 (0.1%)
1	B	0.53	0/3131	0.73	2/4256 (0.0%)
1	C	0.49	0/3131	0.74	1/4256 (0.0%)
1	D	0.47	0/3131	0.72	3/4256 (0.1%)
2	I	0.62	0/104	0.59	0/136
All	All	0.50	0/12628	0.73	9/17160 (0.1%)

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	I	0	2

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	234	LEU	N-CA-C	-6.30	93.98	111.00
1	C	234	LEU	N-CA-C	-6.17	94.33	111.00
1	A	342	TYR	N-CA-C	-5.82	95.29	111.00
1	B	234	LEU	N-CA-C	-5.72	95.55	111.00
1	D	198	TYR	N-CA-C	-5.59	95.91	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	10	STA	Mainchain,Peptide

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	3053	0	2965	54	0
1	B	3053	0	2965	53	0
1	C	3053	0	2965	53	0
1	D	3053	0	2965	57	0
2	I	116	0	114	13	0
3	A	196	0	0	0	0
3	B	184	0	0	1	0
3	C	190	0	0	2	0
3	D	167	0	0	0	0
3	I	7	0	0	2	0
All	All	13072	0	11974	220	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 10.

The worst 5 of 220 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:B:162:ASN:ND2	1:B:165:GLU:H	1.55	1.04
1:B:314:THR:HG23	1:C:314:THR:HG21	1.40	1.00
1:C:73:GLN:HG2	2:I:9:ASN:HB2	1.46	0.94
1:C:234:LEU:HG	1:C:337:ILE:HD11	1.52	0.89
1:D:312:VAL:HG23	1:D:313:ALA:H	1.40	0.86

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	387/389 (100%)	367 (95%)	16 (4%)	4 (1%)	15	9
1	B	387/389 (100%)	372 (96%)	12 (3%)	3 (1%)	19	13
1	C	387/389 (100%)	370 (96%)	12 (3%)	5 (1%)	12	6
1	D	387/389 (100%)	371 (96%)	12 (3%)	4 (1%)	15	9
2	I	11/14 (79%)	8 (73%)	2 (18%)	1 (9%)	1	0
All	All	1559/1570 (99%)	1488 (95%)	54 (4%)	17 (1%)	14	8

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	LYS
1	A	223	ASP
1	A	312	VAL
1	A	314	THR
1	B	75	LYS

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	331/331 (100%)	324 (98%)	7 (2%)	53	57
1	B	331/331 (100%)	320 (97%)	11 (3%)	38	37
1	C	331/331 (100%)	323 (98%)	8 (2%)	49	51
1	D	331/331 (100%)	319 (96%)	12 (4%)	35	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	12/12 (100%)	10 (83%)	2 (17%)	2	1
All	All	1336/1336 (100%)	1296 (97%)	40 (3%)	41	41

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	30	LEU
1	C	197	TRP
1	D	336	VAL
1	C	149	LEU
1	C	209	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	304	GLN
1	C	73	GLN
1	D	304	GLN
1	B	362	HIS
1	C	111	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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
2	STA	I	10	2	10,10,11	0.91	1 (10%)	9,12,14	0.74	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	STA	I	10	2	-	3/11/11/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	10	STA	CH-CA	2.39	1.55	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	10	STA	N-CA-CB-CG
2	I	10	STA	O-C-CM-CH
2	I	10	STA	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.