



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 13, 2016 – 02:32 PM EST

PDB ID : 5FN2  
EMDB ID: : EMD-3237  
Title : Cryo-EM structure of gamma secretase in complex with a drug DAPT  
Authors : Bai, X.C.; Rajendra, E.; Yang, G.H.; Shi, Y.G.; Scheres, S.H.W.  
Deposited on : 2015-11-10  
Resolution : 4.20 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

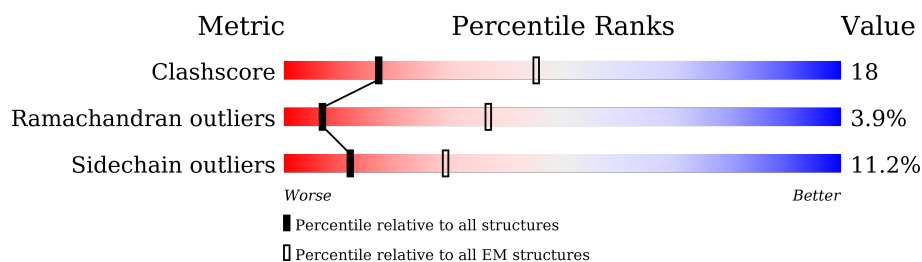
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	709	
2	B	467	
3	C	265	
4	D	101	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10276 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 NICASTRIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	665	Total	C	N	O	S	0	0
			5222	3312	888	1001	21		

- Molecule 2 is a protein called PRESENILIN-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	301	Total	C	N	O	S	0	0
			2339	1590	354	381	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	256	THR	TYR	CONFLICT	UNP P49768

- Molecule 3 is a protein called GAMMA-SECRETASE SUBUNIT APH-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	243	Total	C	N	O	S	0	0
			1868	1252	299	313	4		

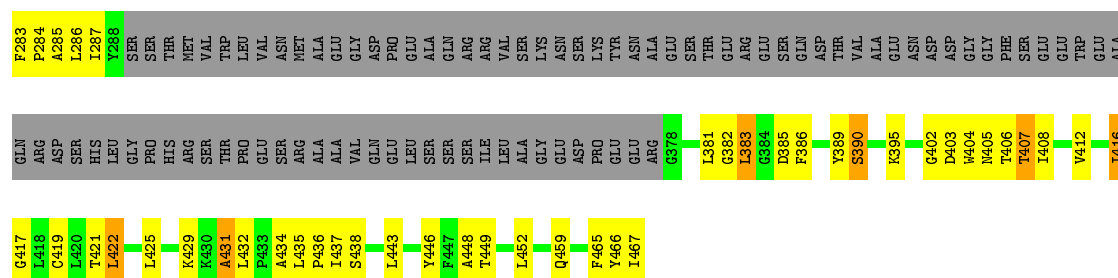
- Molecule 4 is a protein called GAMMA-SECRETASE SUBUNIT PEN-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	100	Total	C	N	O	S	0	0
			847	579	133	134	1		

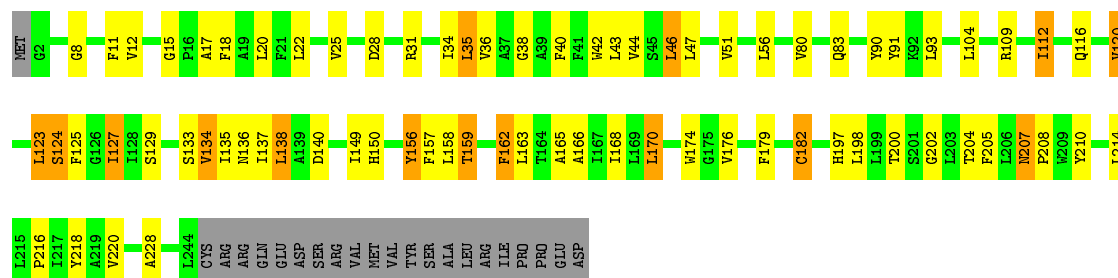


- Molecule 1: NICASTRIN

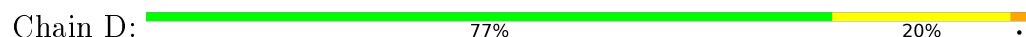




• Molecule 3: GAMMA-SECRETASE SUBUNIT APH-1A



• Molecule 4: GAMMA-SECRETASE SUBUNIT PEN-2



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	51366	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	38	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 QUANTUM (4K X 4K)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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  >2	RMSZ	# Z  >2
1	A	0.47	0/5345	0.79	4/7284 (0.1%)
2	B	0.54	0/2399	0.90	1/3279 (0.0%)
3	C	0.54	0/1920	0.89	0/2619
4	D	0.52	0/880	0.76	0/1201
All	All	0.51	0/10544	0.83	5/14383 (0.0%)

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
1	A	0	5
2	B	0	2
All	All	0	7

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	PHE	CB-CG-CD1	7.91	126.33	120.80
1	A	218	PHE	CB-CG-CD2	-6.38	116.34	120.80
1	A	312	LEU	CA-CB-CG	5.51	127.98	115.30
2	B	263	CYS	C-N-CD	5.37	139.67	128.40
1	A	218	PHE	N-CA-CB	5.26	120.07	110.60

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	LEU	Peptide
1	A	256	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	288	PHE	Peptide
1	A	335	PHE	Peptide
1	A	91	ASN	Peptide

## 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	5222	0	5120	113	0
2	B	2339	0	2453	214	0
3	C	1868	0	1907	55	0
4	D	847	0	836	16	0
All	All	10276	0	10316	372	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 18.

The worst 5 of 372 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:B:114:ILE:O	2:B:117:PRO:HD2	1.38	1.24
2:B:263:CYS:O	2:B:267:PRO:HD2	1.38	1.20
2:B:113:LEU:HD23	2:B:240:TYR:O	1.44	1.17
2:B:141:SER:O	2:B:145:VAL:HG23	1.47	1.13
2:B:144:VAL:O	2:B:147:THR:HG22	1.44	1.12

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 PDB entries followed by that with respect to all EM entries.

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	663/709 (94%)	528 (80%)	102 (15%)	33 (5%)	3	31
2	B	297/467 (64%)	262 (88%)	20 (7%)	15 (5%)	2	31
3	C	241/265 (91%)	217 (90%)	22 (9%)	2 (1%)	24	69
4	D	98/101 (97%)	86 (88%)	11 (11%)	1 (1%)	19	65
All	All	1299/1542 (84%)	1093 (84%)	155 (12%)	51 (4%)	7	37

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	TRP
1	A	333	GLU
1	A	422	LEU
1	A	472	SER
1	A	475	GLU

### 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 PDB entries followed by that with respect to all EM entries.

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	583/612 (95%)	529 (91%)	54 (9%)	11	46
2	B	250/408 (61%)	208 (83%)	42 (17%)	2	20
3	C	192/214 (90%)	170 (88%)	22 (12%)	7	36
4	D	87/89 (98%)	80 (92%)	7 (8%)	15	53
All	All	1112/1323 (84%)	987 (89%)	125 (11%)	12	37

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	92	CYS
2	B	171	LEU
3	C	182	CYS

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Mol	Chain	Res	Type
2	B	110	ASP
2	B	146	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	462	ASN
3	C	207	ASN
2	B	135	ASN
1	A	142	ASN
1	A	596	ASN

### 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](#)

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.