



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 13, 2016 – 02:17 PM EST

PDB ID : 5FN3
EMDB ID: : EMD-3238
Title : Cryo-EM structure of gamma secretase in class 1 of the apo- state ensemble
Authors : Bai, X.C.; Rajendra, E.; Yang, G.H.; Shi, Y.G.; Scheres, S.H.W.
Deposited on : 2015-11-10
Resolution : 4.10 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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

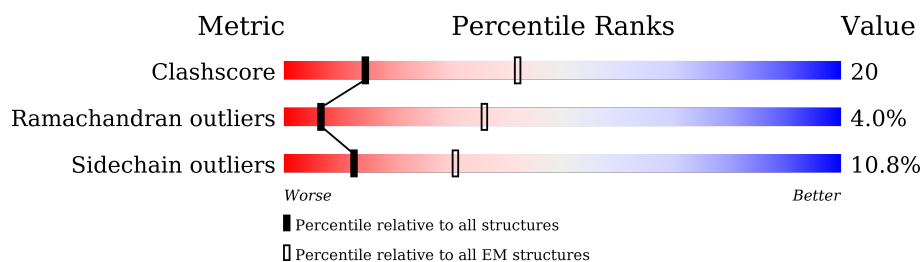
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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 ≥ 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	69% 21% • 6%
2	B	467	28% 25% 7% • 39%
3	C	265	62% 27% • 8%
4	D	101	78% 19% ••
5	G	24	38% 33% 25% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10291 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	286	Total	C	N	O	S	0	0
			2234	1523	335	363	13		

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.

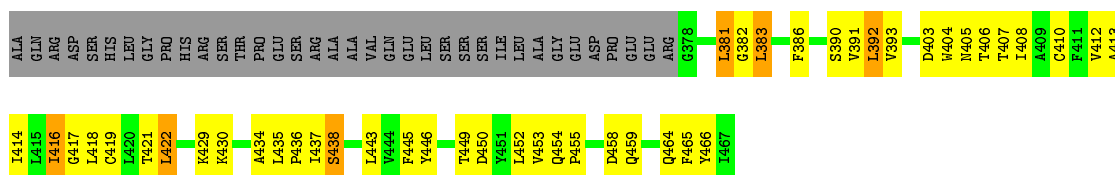
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	243	Total	C	N	O	S	0	0
			1868	1252	299	313	4		

- 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		

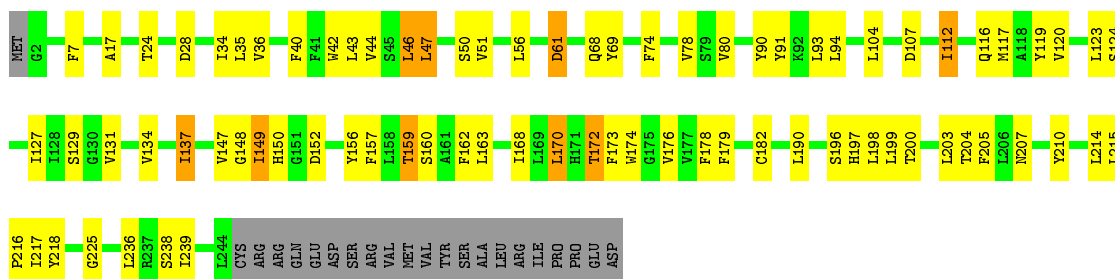
- Molecule 5 is a protein called POLY ALA CHAIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	24	Total	C	N	O	0	0
			120	72	24	24		



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

Chain C: 62% 27% 8%



• Molecule 4: GAMMA-SECRETASE SUBUNIT PEN-2

Chain D: 78% 19% 2%



• Molecule 5: POLY ALA CHAIN

Chain G: 38% 33% 25%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	63873	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)	700	Depositor
Maximum defocus (nm)	3200	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	0.52	1/5345 (0.0%)	0.81	2/7284 (0.0%)
2	B	0.66	1/2291 (0.0%)	0.98	5/3130 (0.2%)
3	C	0.65	0/1920	0.95	2/2619 (0.1%)
4	D	0.66	0/880	0.82	0/1201
5	G	0.20	0/119	0.34	0/165
All	All	0.59	2/10555 (0.0%)	0.87	9/14399 (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
1	A	0	5
2	B	0	15
5	G	0	8
All	All	0	28

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	TRP	CB-CG	-5.53	1.40	1.50
2	B	244	TRP	CB-CG	5.17	1.59	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	117	PRO	CA-N-CD	-7.03	101.66	111.50
3	C	47	LEU	CA-CB-CG	6.85	131.04	115.30
3	C	69	TYR	CA-CB-CG	6.14	125.07	113.40
2	B	116	THR	C-N-CD	5.95	140.89	128.40
1	A	312	LEU	CA-CB-CG	5.46	127.87	115.30

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	VAL	Peptide
1	A	335	PHE	Peptide
1	A	57	THR	Peptide
1	A	62	CYS	Peptide
1	A	622	ARG	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	5222	0	5120	91	0
2	B	2234	0	2344	261	0
3	C	1868	0	1907	54	0
4	D	847	0	836	11	0
5	G	120	0	119	59	0
All	All	10291	0	10326	412	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 20.

The worst 5 of 412 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)
5:G:15:ALA:C	5:G:17:ALA:HB3	1.31	1.42
2:B:112:GLN:CD	5:G:15:ALA:HB2	1.61	1.20
5:G:15:ALA:O	5:G:17:ALA:CB	1.89	1.19
2:B:146:MET:CE	5:G:25:ALA:H	1.56	1.18
2:B:146:MET:HE1	5:G:25:ALA:N	1.58	1.17

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 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%)	534 (80%)	99 (15%)	30 (4%)	3	34
2	B	280/467 (60%)	248 (89%)	16 (6%)	16 (6%)	2	29
3	C	241/265 (91%)	221 (92%)	16 (7%)	4 (2%)	11	56
4	D	98/101 (97%)	89 (91%)	8 (8%)	1 (1%)	19	65
5	G	22/24 (92%)	20 (91%)	1 (4%)	1 (4%)	3	34
All	All	1304/1566 (83%)	1112 (85%)	140 (11%)	52 (4%)	6	37

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
1	A	333	GLU
1	A	473	PRO
1	A	643	THR
2	B	116	THR

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%)	530 (91%)	53 (9%)	12	47
2	B	240/408 (59%)	206 (86%)	34 (14%)	4	28
3	C	192/214 (90%)	170 (88%)	22 (12%)	7	36
4	D	87/89 (98%)	77 (88%)	10 (12%)	7	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1102/1323 (83%)	983 (89%)	119 (11%)	12	39

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	80	LYS
2	B	184	GLU
4	D	17	LYS
2	B	87	VAL
2	B	133	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	GLN
1	A	606	GLN
2	B	464	GLN
1	A	450	ASN
2	B	454	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

There are no ligands in this entry.

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.