



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 19, 2016 – 07:49 PM EST

PDB ID : 5A63
EMDB ID: : EMD-3061
Title : Cryo-EM structure of the human gamma-secretase complex at 3.4 angstrom resolution.
Authors : Bai, X.; Yan, C.; Yang, G.; Lu, P.; Ma, D.; Sun, L.; Zhou, R.; Scheres, S.H.W.; Shi, Y.
Deposited on : 2015-06-24
Resolution : 3.40 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 : 1.7.1 (RC1), CSD as537be (2016)
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

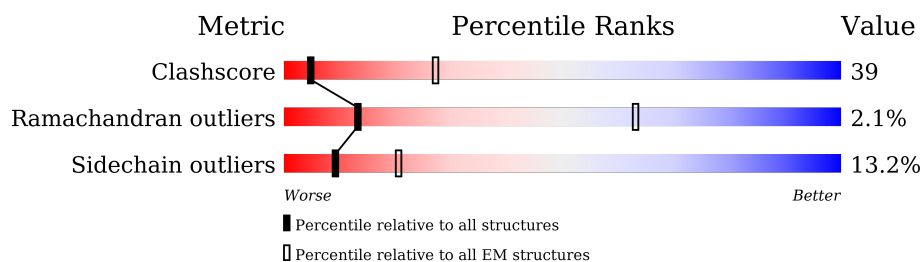
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	
2	B	467	
3	C	265	
4	D	101	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10003 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	215	Total	C	N	O	S	0	0
			1702	1170	249	274	9		

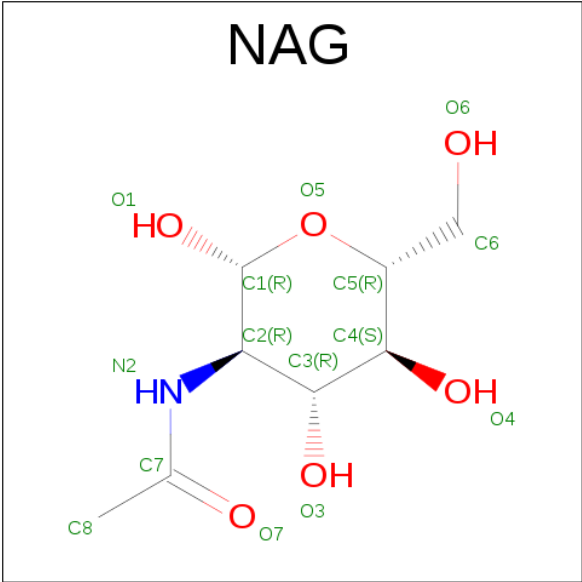
- Molecule 3 is a protein called GAMMA-SECRETASE SUBUNIT APH-1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	243	Total	C	N	O	S	0	0
			1872	1254	299	315	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
			850	580	134	135	1		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



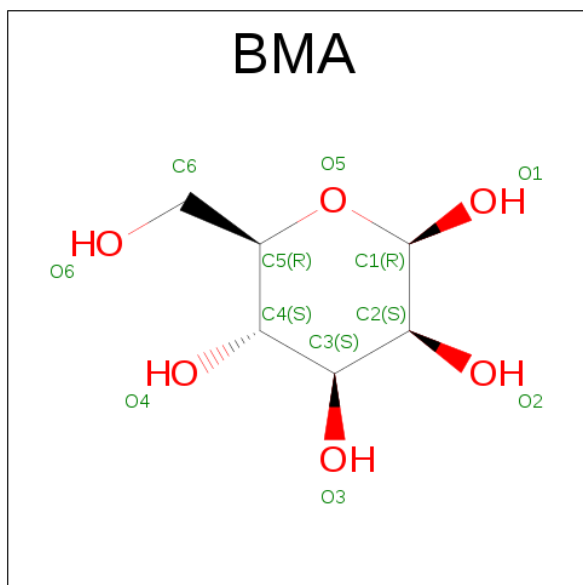
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	

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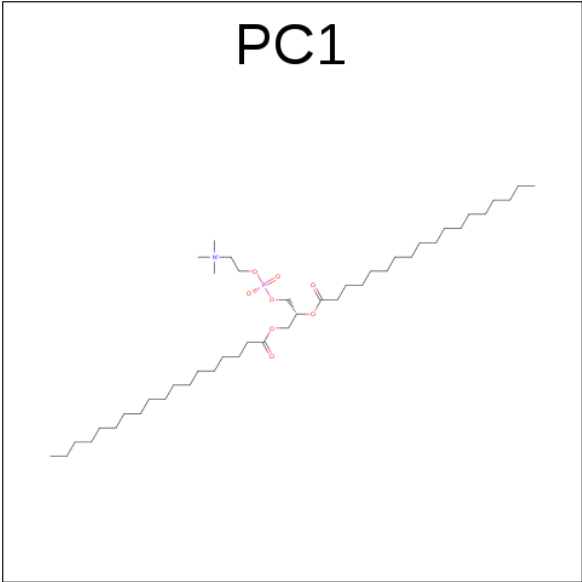
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	
5	A	1	Total	C	N	O	0
			238	136	17	85	

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			33	18	15	
6	A	1	Total	C	O	0
			33	18	15	
6	A	1	Total	C	O	0
			33	18	15	

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).

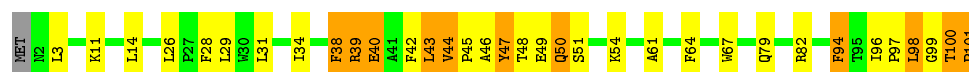


Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			43	33	1	8	1	
7	C	1	Total	C	N	O	P	0
			43	33	1	8	1	

i

- Molecule 1: NICASTRIN





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	159549	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	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 (4K X 4K)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, PC1

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	0.54	3/5345 (0.1%)	0.75	8/7284 (0.1%)
2	B	0.46	1/1748 (0.1%)	0.76	1/2385 (0.0%)
3	C	0.48	1/1924 (0.1%)	0.78	1/2624 (0.0%)
4	D	0.53	1/883 (0.1%)	0.74	2/1205 (0.2%)
All	All	0.51	6/9900 (0.1%)	0.76	12/13498 (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	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	PRO	N-CD	5.29	1.55	1.47
1	A	608	PRO	N-CD	5.28	1.55	1.47
1	A	421	PRO	N-CD	5.23	1.55	1.47
3	C	111	PRO	N-CD	5.17	1.55	1.47
4	D	101	PRO	N-CD	5.13	1.55	1.47

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	SER	C-N-CD	6.60	142.25	128.40
1	A	423	PRO	C-N-CD	6.05	141.11	128.40
1	A	632	SER	C-N-CD	5.90	140.78	128.40
1	A	422	LEU	C-N-CD	5.81	140.61	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	44	VAL	C-N-CD	5.79	140.57	128.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	PHE	Peptide
1	A	256	VAL	Peptide
1	A	68	GLY	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	5113	562	0
2	B	1702	0	1793	107	0
3	C	1872	0	1911	88	0
4	D	850	0	840	50	0
5	A	238	0	214	6	0
6	A	33	0	28	0	0
7	B	43	0	60	0	0
7	C	43	0	60	1	0
All	All	10003	0	10019	772	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 39.

The worst 5 of 772 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:A:316:PRO:HG2	1:A:507:PHE:CD2	1.52	1.42
1:A:152:TYR:CE1	1:A:383:VAL:HG21	1.61	1.36
1:A:279:ALA:O	1:A:364:GLU:HG2	1.29	1.28
1:A:633:PRO:HB2	1:A:645:TYR:CD2	1.66	1.28
1:A:155:GLU:HG3	1:A:156:PHE:CE1	1.71	1.24

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%)	589 (89%)	54 (8%)	20 (3%)	5	39
2	B	209/467 (45%)	196 (94%)	8 (4%)	5 (2%)	7	44
3	C	241/265 (91%)	228 (95%)	12 (5%)	1 (0%)	39	79
4	D	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
All	All	1211/1542 (78%)	1108 (92%)	77 (6%)	26 (2%)	13	47

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	SER
1	A	559	SER
1	A	210	PHE
1	A	333	GLU
1	A	371	ARG

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 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%)	497 (85%)	86 (15%)	4	20
2	B	184/408 (45%)	165 (90%)	19 (10%)	9	37
3	C	193/214 (90%)	171 (89%)	22 (11%)	7	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	88/89 (99%)	77 (88%)	11 (12%)	6	27
All	All	1048/1323 (79%)	910 (87%)	138 (13%)	9	25

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	LEU
1	A	624	THR
4	D	14	LEU
1	A	436	ILE
1	A	561	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	393	GLN
1	A	478	ASN
4	D	8	ASN
1	A	418	GLN
1	A	428	GLN

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](#)

22 ligands are 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
5	NAG	A	1699	1,5	14,14,15	0.56	0	15,19,21	1.01	1 (6%)
5	NAG	A	1700	5	14,14,15	0.50	0	15,19,21	1.23	2 (13%)
5	NAG	A	1701	1,5	14,14,15	0.48	0	15,19,21	1.56	2 (13%)
5	NAG	A	1702	5,6	14,14,15	0.47	0	15,19,21	0.82	0
5	NAG	A	1703	1,5	14,14,15	0.60	0	15,19,21	1.31	1 (6%)
5	NAG	A	1704	5	14,14,15	0.55	0	15,19,21	1.33	2 (13%)
5	NAG	A	1705	1	14,14,15	0.53	0	15,19,21	0.82	0
5	NAG	A	1706	1,5	14,14,15	0.48	0	15,19,21	1.11	2 (13%)
5	NAG	A	1707	5	14,14,15	0.52	0	15,19,21	1.17	3 (20%)
5	NAG	A	1708	1,5	14,14,15	0.50	0	15,19,21	0.98	1 (6%)
5	NAG	A	1709	5	14,14,15	0.70	0	15,19,21	2.24	5 (33%)
5	NAG	A	1710	1,5	14,14,15	0.65	0	15,19,21	1.31	1 (6%)
5	NAG	A	1711	5	14,14,15	0.47	0	15,19,21	0.70	0
5	NAG	A	1712	1	14,14,15	0.44	0	15,19,21	0.74	0
5	NAG	A	1713	1	14,14,15	0.51	0	15,19,21	0.83	0
5	NAG	A	1714	1	14,14,15	0.48	0	15,19,21	0.68	0
5	NAG	A	1715	1	14,14,15	0.46	0	15,19,21	0.74	0
6	BMA	A	1716	5,6	11,11,12	0.38	0	15,15,17	0.96	1 (6%)
6	BMA	A	1717	6	11,11,12	0.39	0	15,15,17	1.57	3 (20%)
6	BMA	A	1718	6	11,11,12	0.31	0	15,15,17	0.64	0
7	PC1	B	1468	-	42,42,53	1.03	2 (4%)	46,50,61	1.04	2 (4%)
7	PC1	C	1245	-	42,42,53	1.05	2 (4%)	46,50,61	1.00	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
5	NAG	A	1699	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1700	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1701	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1702	5,6	-	0/6/23/26	0/1/1/1
5	NAG	A	1703	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1704	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1705	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1706	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1707	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1708	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1709	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1710	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1711	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1712	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1713	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1714	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1715	1	-	0/6/23/26	0/1/1/1
6	BMA	A	1716	5,6	-	0/2/19/22	0/1/1/1
6	BMA	A	1717	6	-	0/2/19/22	0/1/1/1
6	BMA	A	1718	6	-	0/2/19/22	0/1/1/1
7	PC1	B	1468	-	-	0/46/46/57	0/0/0/0
7	PC1	C	1245	-	-	0/46/46/57	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1468	PC1	O21-C21	4.11	1.46	1.34
7	C	1245	PC1	O21-C21	4.21	1.46	1.34
7	B	1468	PC1	O31-C31	4.25	1.46	1.33
7	C	1245	PC1	O31-C31	4.36	1.46	1.33

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1710	NAG	O5-C5-C4	-3.57	104.23	110.13
5	A	1709	NAG	O7-C7-C8	-2.79	116.93	122.07
5	A	1706	NAG	C4-C3-C2	-2.22	107.90	111.34
5	A	1708	NAG	C4-C3-C2	2.02	114.48	111.34
5	A	1707	NAG	C1-O5-C5	2.05	115.16	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1705	NAG	2	0
5	A	1706	NAG	1	0
5	A	1707	NAG	1	0
5	A	1710	NAG	2	0
5	A	1714	NAG	1	0
7	C	1245	PC1	1	0

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.