



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:59 PM BST

PDB ID : 4UIS  
EMDB ID: : EMD-2974  
Title : The cryoEM structure of human gamma-Secretase complex  
Authors : Sun, L.; Zhao, L.; Yang, G.; Yan, C.; Zhou, R.; Zhou, X.; Xie, T.; Zhao, Y.;  
Wu, S.; Li, X.; Shi, Y.  
Deposited on : 2015-04-03  
Resolution : 4.40 Å(reported)  
Based on PDB ID : 4R12

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could  
stem from errors in the original structure(s) used in the fitting.  
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>

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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) : trunk27241

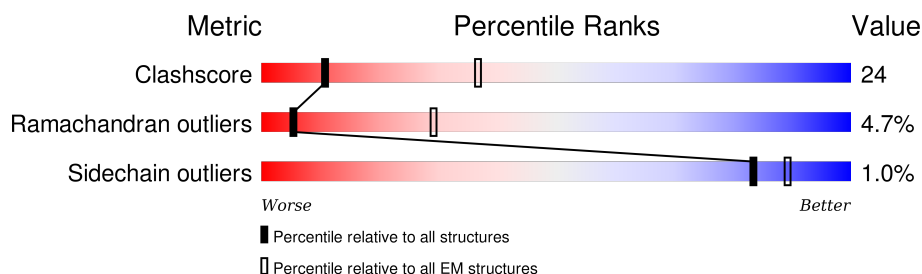
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 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  $\geq 3$ , 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	588	51% 44% .
2	B	241	78% 21% .
3	C	196	98% .
4	D	62	100%
5	G	162	59% 41%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8518 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 GAMMA-SECRETASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	588	Total	C	N	O	S	0	0
			4372	2761	758	835	18		

- Molecule 2 is a protein called GAMMA-SECRETASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	241	Total	C	N	O	S	0	0
			1522	987	257	271	7		

- Molecule 3 is a protein called GAMMA-SECRETASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	196	Total	C	N	O	0	0
			969	577	196	196		

- Molecule 4 is a protein called GAMMA-SECRETASE.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	62	Total	C	N	O	0	0
			306	182	62	62		

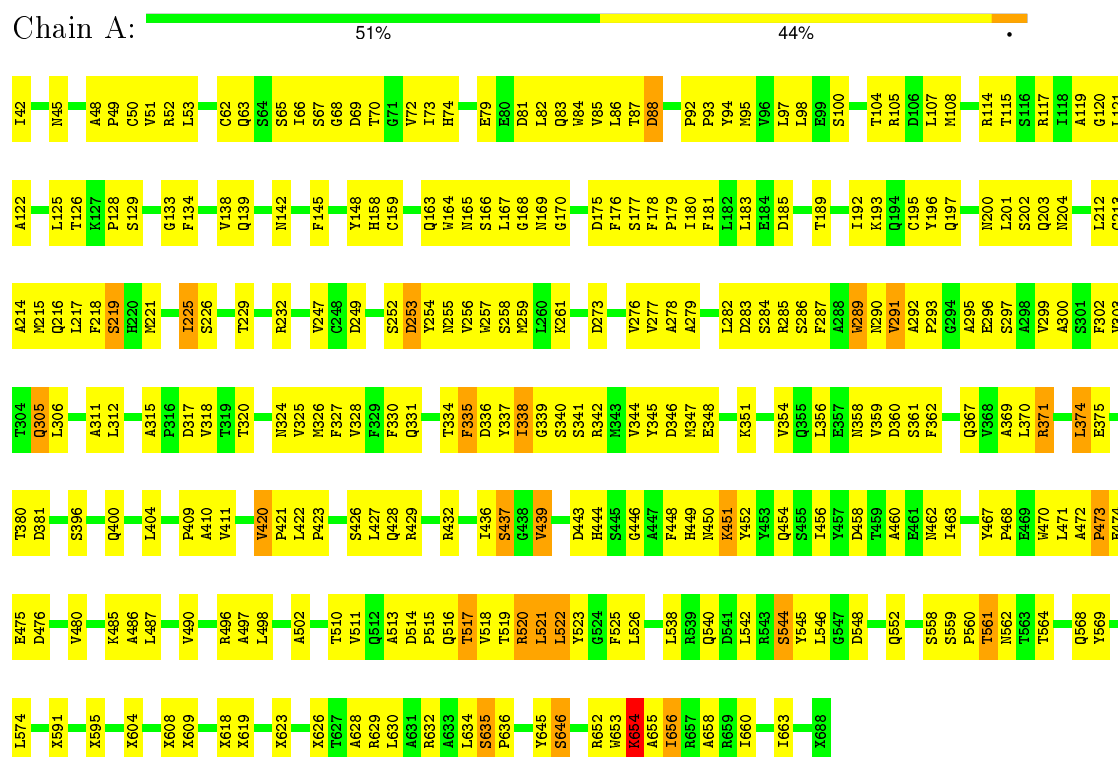
- Molecule 5 is a protein called LYSOZYME.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	162	Total	C	N	O	S	6	0
			1349	845	250	247	7		

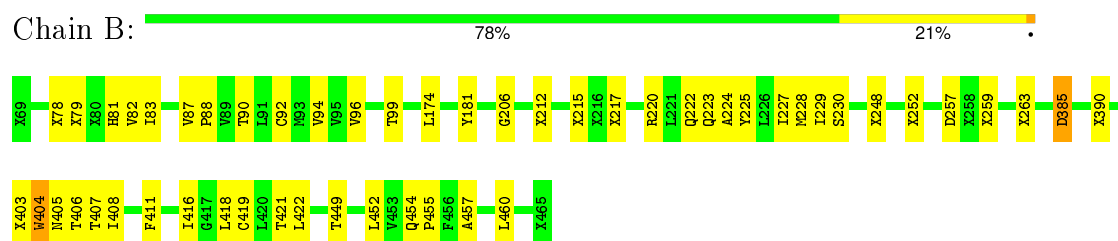
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

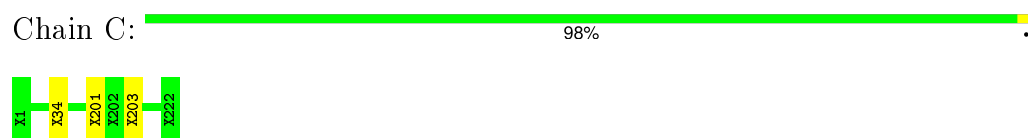
#### • Molecule 1: GAMMA-SECRETASE



#### • Molecule 2: GAMMA-SECRETASE



#### • Molecule 3: GAMMA-SECRETASE



● Molecule 4: GAMMA-SECRETASE

Chain D: 

100%

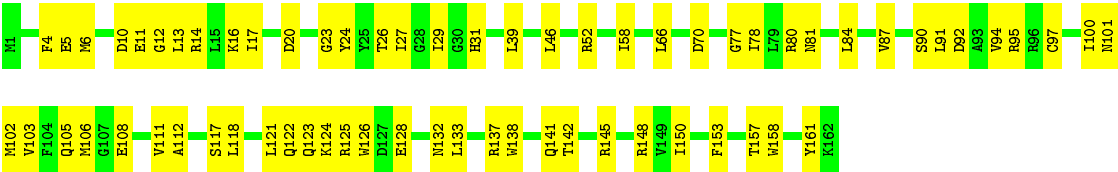
There are no outlier residues recorded for this chain.

● Molecule 5: LYSOZYME

Chain G: 

59%

41%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	4.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	DIRECT ELECTRON DE-12 (4K X 3K)	Depositor

## 5 Model quality [i](#)

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

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	0.46	0/4153	0.65	0/5654
2	B	0.44	0/844	0.60	1/1142 (0.1%)
5	G	0.26	0/1361	0.47	0/1816
All	All	0.42	0/6358	0.61	1/8612 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	385	ASP	CB-CG-OD2	5.22	123.00	118.30

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	4372	0	4041	281	0
2	B	1522	0	1007	31	0
3	C	969	0	197	2	0
4	D	306	0	63	0	0
5	G	1349	0	1363	54	0
All	All	8518	0	6671	367	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 24.

The worst 5 of 367 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:219:SER:CB	1:A:656:ILE:CG2	1.91	1.49
1:A:467:TYR:HE2	1:A:523:TYR:CE2	1.31	1.46
1:A:522:LEU:HD11	1:A:526:LEU:CD1	1.45	1.46
1:A:467:TYR:CE2	1:A:523:TYR:HE2	1.36	1.41
1:A:219:SER:HB2	1:A:656:ILE:CG2	1.44	1.38

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	509/588 (87%)	425 (84%)	48 (9%)	36 (7%)	1	23
2	B	102/241 (42%)	96 (94%)	6 (6%)	0	100	100
5	G	152/162 (94%)	147 (97%)	5 (3%)	0	100	100
All	All	763/991 (77%)	668 (88%)	59 (8%)	36 (5%)	5	33

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	ASP
1	A	289	TRP
1	A	291	VAL
1	A	436	ILE
1	A	635	SER

### 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	441/448 (98%)	435 (99%)	6 (1%)	74	89
2	B	90/90 (100%)	89 (99%)	1 (1%)	80	90
5	G	142/136 (104%)	142 (100%)	0	100	100
All	All	673/674 (100%)	666 (99%)	7 (1%)	83	91

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	522	LEU
2	B	404	TRP
1	A	654	LYS
1	A	520	ARG
1	A	656	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	ASN
1	A	568	GLN
1	A	290	ASN
1	A	216	GLN
1	A	450	ASN

### 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 [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.