



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:33 pm GMT

PDB ID : 2Q11
Title : Structure of BACE complexed to compound 1
Authors : Sharff, A.J.
Deposited on : 2007-05-23
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

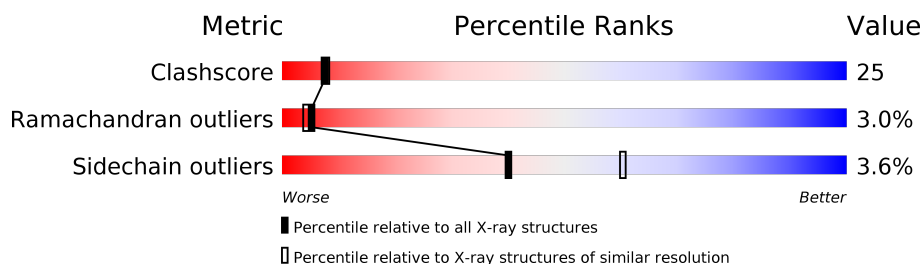
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	
1	B	388	
1	C	388	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9647 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.

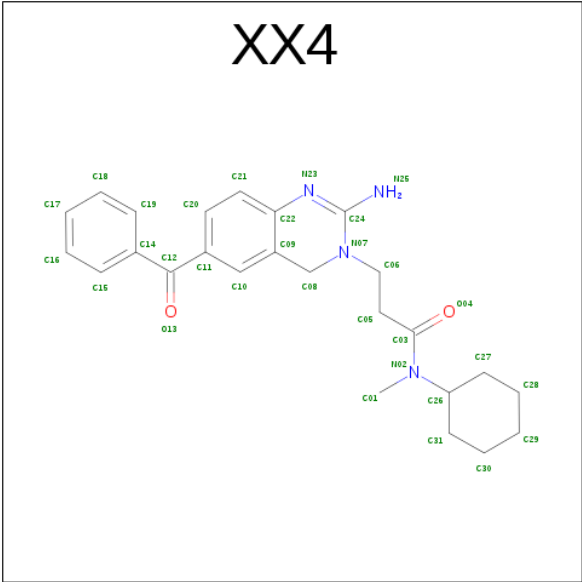
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	164	0	0
			3049	1952	505	578	14			
1	B	388	Total	C	N	O	S	164	0	0
			3053	1955	506	578	14			
1	C	388	Total	C	N	O	S	164	0	0
			3045	1950	504	577	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLN	ASN	ENGINEERED	UNP P56817
A	111	GLN	ASN	ENGINEERED	UNP P56817
A	162	GLN	ASN	ENGINEERED	UNP P56817
A	293	GLN	ASN	ENGINEERED	UNP P56817
B	92	GLN	ASN	ENGINEERED	UNP P56817
B	111	GLN	ASN	ENGINEERED	UNP P56817
B	162	GLN	ASN	ENGINEERED	UNP P56817
B	293	GLN	ASN	ENGINEERED	UNP P56817
C	92	GLN	ASN	ENGINEERED	UNP P56817
C	111	GLN	ASN	ENGINEERED	UNP P56817
C	162	GLN	ASN	ENGINEERED	UNP P56817
C	293	GLN	ASN	ENGINEERED	UNP P56817

- Molecule 2 is 3-(2-AMINO-6-BENZOYLQUINAZOLIN-3(4H)-YL)-N-CYCLOHEXYL-N-METHYLPROPANAMIDE (three-letter code: XX4) (formula: C₂₅H₃₀N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	25	4	2		
2	B	1	Total	C	N	O	0	0
			31	25	4	2		
2	C	1	Total	C	N	O	0	0
			31	25	4	2		

- Molecule 3 is water.

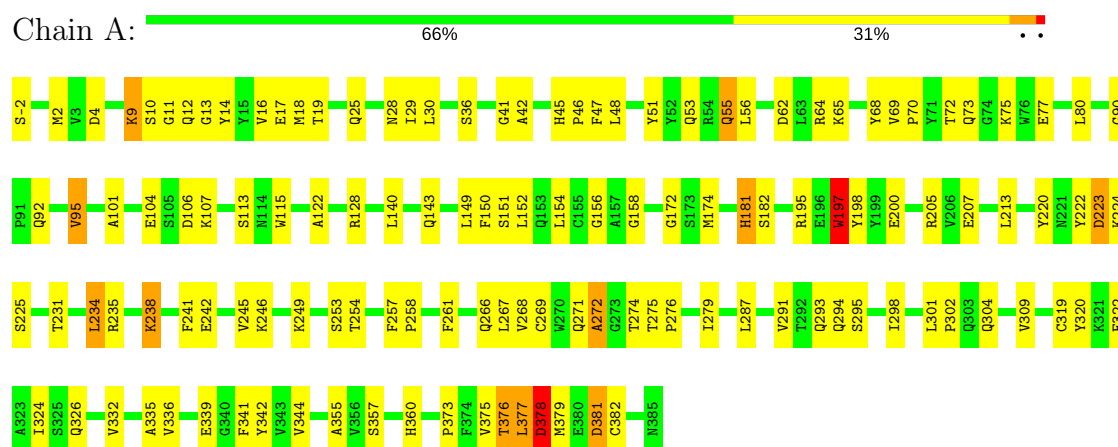
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	155	Total	O	0	0
			155	155		
3	B	123	Total	O	0	0
			123	123		
3	C	129	Total	O	0	0
			129	129		

3 Residue-property plots

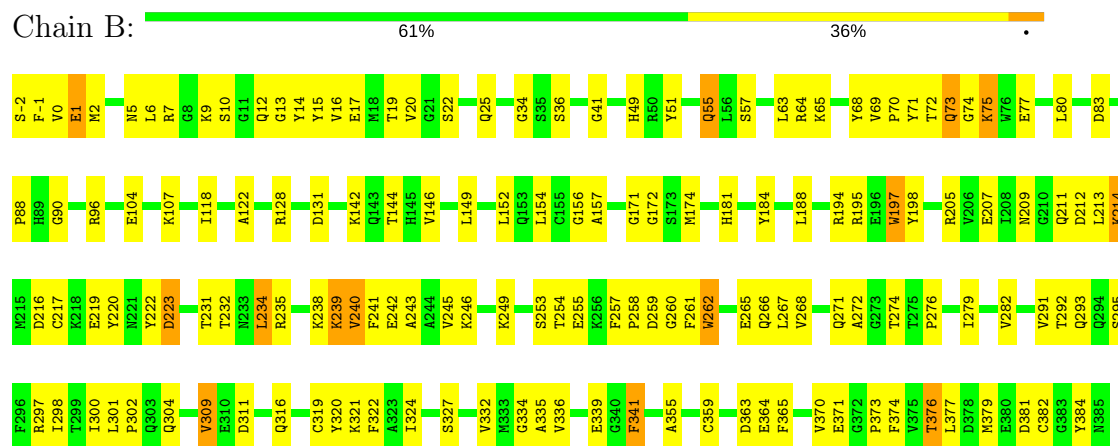
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

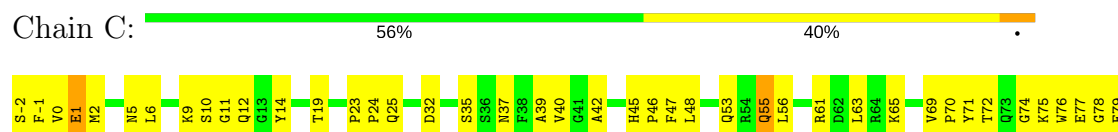
• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1





4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	235.90Å 108.50Å 63.10Å 90.00° 102.94° 90.00°	Depositor
Resolution (Å)	500.00 – 2.40	Depositor
% Data completeness (in resolution range)	97.9 (500.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.278 , 0.337	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9647	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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: XX4

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	0.41	0/3127	0.68	2/4251 (0.0%)
1	B	0.37	0/3131	0.64	0/4255
1	C	0.39	0/3123	0.63	1/4246 (0.0%)
All	All	0.39	0/9381	0.65	3/12752 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	342	TYR	N-CA-C	-5.28	96.74	111.00
1	A	342	TYR	N-CA-C	-5.20	96.95	111.00
1	A	197	TRP	N-CA-C	-5.13	97.14	111.00

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	3049	0	2956	124	0
1	B	3053	0	2967	145	0
1	C	3045	0	2950	161	0
2	A	31	0	30	4	0
2	B	31	0	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	30	6	0
3	A	155	0	0	5	0
3	B	123	0	0	8	0
3	C	129	0	0	7	0
All	All	9647	0	8963	424	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 25.

The worst 5 of 424 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:C:267:LEU:HD22	1:C:309:VAL:HG21	1.32	1.09
1:B:301:LEU:H	1:B:304:GLN:NE2	1.70	0.89
1:B:276:PRO:O	1:B:279:ILE:HG12	1.77	0.84
1:C:75:LYS:HA	2:C:503:XX4:H18	1.60	0.83
1:A:9:LYS:HE2	1:A:11:GLY:H	1.43	0.82

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	386/388 (100%)	343 (89%)	37 (10%)	6 (2%)	11	15
1	B	386/388 (100%)	328 (85%)	42 (11%)	16 (4%)	3	2
1	C	386/388 (100%)	340 (88%)	33 (8%)	13 (3%)	4	3
All	All	1158/1164 (100%)	1011 (87%)	112 (10%)	35 (3%)	5	4

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	A	377	LEU
1	B	157	ALA
1	B	223	ASP
1	B	240	VAL

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 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	330/331 (100%)	319 (97%)	11 (3%)	43	64
1	B	331/331 (100%)	321 (97%)	10 (3%)	46	67
1	C	329/331 (99%)	314 (95%)	15 (5%)	31	49
All	All	990/993 (100%)	954 (96%)	36 (4%)	40	60

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	197	TRP
1	B	381	ASP
1	C	336	VAL
1	B	262	TRP
1	C	1	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	28	ASN
1	B	304	GLN
1	C	271	GLN
1	A	362	HIS
1	C	55	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 ⓘ

3 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$
2	XX4	A	501	-	34,34,34	1.82	9 (26%)	43,47,47	1.10	3 (6%)
2	XX4	B	502	-	34,34,34	1.82	9 (26%)	43,47,47	1.06	2 (4%)
2	XX4	C	503	-	34,34,34	1.69	8 (23%)	43,47,47	1.17	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
2	XX4	A	501	-	-	0/21/41/41	0/4/4/4
2	XX4	B	502	-	-	0/21/41/41	0/4/4/4
2	XX4	C	503	-	-	0/21/41/41	0/4/4/4

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	XX4	C21-C22	2.04	1.43	1.40
2	C	503	XX4	C20-C11	2.27	1.43	1.39
2	B	502	XX4	C24-N07	2.53	1.40	1.35
2	A	501	XX4	C24-N25	2.58	1.39	1.34
2	B	502	XX4	C19-C14	2.59	1.43	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	XX4	N07-C24-N23	-4.12	120.02	125.43
2	A	501	XX4	N07-C24-N23	-3.60	120.70	125.43
2	C	503	XX4	N07-C24-N23	-2.91	121.61	125.43
2	A	501	XX4	C09-C22-N23	-2.02	120.16	122.11
2	B	502	XX4	C22-N23-C24	3.27	121.26	117.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	XX4	4	0
2	B	502	XX4	6	0
2	C	503	XX4	6	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.

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.