wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 09:54 AM EDT

PDB ID	:	1SGZ
Title	:	Crystal Structure of Unbound Beta-Secretase Catalytic Domain.
Authors	:	Hong, L.; Tang, J.
Deposited on	:	2004-02-24
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

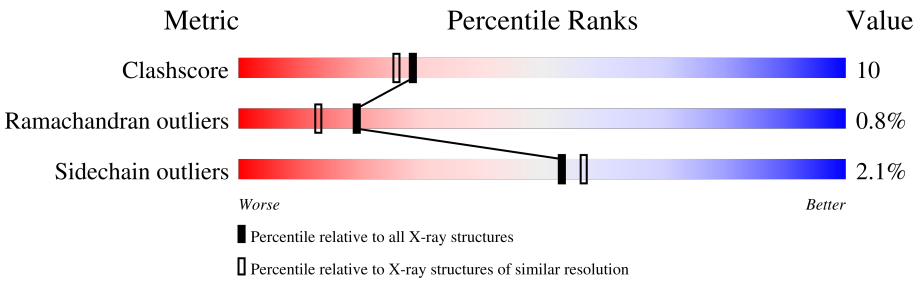
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	389	83% 15% • •
1	B	389	82% 15% •
1	C	389	85% 13% •
1	D	389	81% 16% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13122 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	389	3053	1953	507	579	14	0	0	0
1	B	389	3053	1953	507	579	14	0	0	0
1	C	389	3053	1953	507	579	14	0	0	0
1	D	389	3053	1953	507	579	14	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	234	234	234	0	0
2	B	242	242	242	0	0
2	C	228	228	228	0	0
2	D	206	206	206	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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.

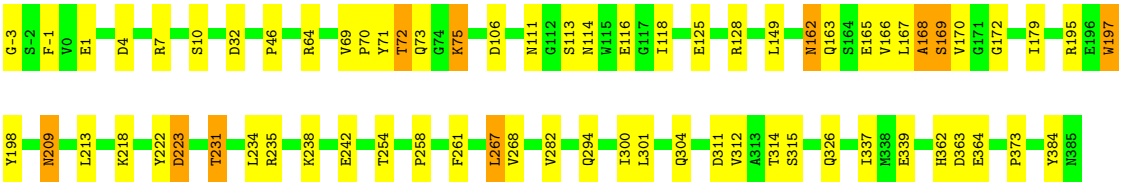
Note EDS was not executed.

• Molecule 1: Beta-secretase

Chain A:

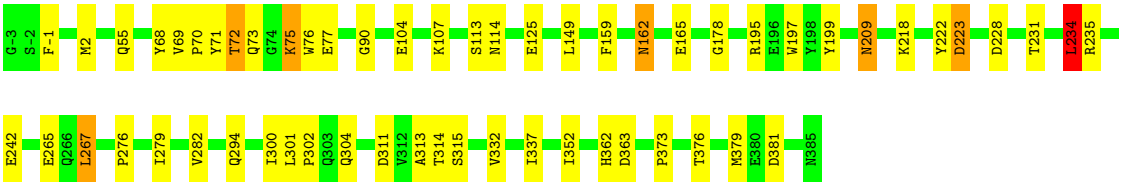
• Molecule 1: Beta-secretase

Chain B:



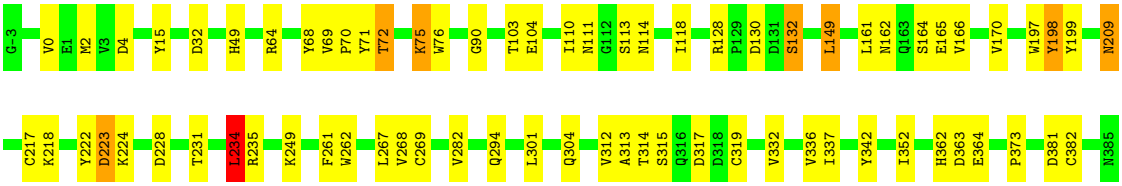
• Molecule 1: Beta-secretase

Chain C:



• Molecule 1: Beta-secretase

Chain D:


G-3
V0
E1
M2
V3
D4
Y15
D32
H49
R64
Y68
V69
P70
Y71
T72
K75
W76
G90
T103
E104
I110
N111
G112
S113
N114
I118
R128
P129
D130
D131
S132
L149
L161
N162
Q163
S164
E165
V166
V170
W197
Y198
Y199
N209
C217
K218
Y222
D223
K224
D228
T231
L234
R235
K249
F261
W262
L267
V268
C269
V282
Q294
L301
Q304
V312
A313
T314
S315
Q316
D317
D318
C319
V332
V336
I337
Y342
I352
H362
D363
E364
P373
D381
C382
N385

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.16Å 130.81Å 88.65Å 90.00° 97.27° 90.00°	Depositor
Resolution (Å)	42.70 – 2.00	Depositor
% Data completeness (in resolution range)	94.6 (42.70-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13122	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

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	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.47	0/3131	0.73	2/4256 (0.0%)
1	B	0.48	0/3131	0.72	1/4256 (0.0%)
1	C	0.46	0/3131	0.73	1/4256 (0.0%)
1	D	0.44	0/3131	0.71	3/4256 (0.1%)
All	All	0.46	0/12524	0.72	7/17024 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	234	LEU	N-CA-C	-6.14	94.43	111.00
1	D	234	LEU	N-CA-C	-6.06	94.64	111.00
1	A	234	LEU	N-CA-C	-5.54	96.03	111.00
1	B	234	LEU	N-CA-C	-5.34	96.57	111.00
1	A	342	TYR	N-CA-C	-5.30	96.70	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	3053	0	2968	57	0
1	B	3053	0	2968	62	0
1	C	3053	0	2968	49	0
1	D	3053	0	2968	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	234	0	0	7	0
2	B	242	0	0	11	0
2	C	228	0	0	2	0
2	D	206	0	0	4	0
All	All	13122	0	11872	221	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 10.

The worst 5 of 221 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:B:70:PRO:HA	1:B:75:LYS:HB3	1.43	1.00
1:B:162:ASN:ND2	1:B:165:GLU:H	1.70	0.89
1:D:267:LEU:H	1:D:267:LEU:HD23	1.39	0.86
1:C:70:PRO:HA	1:C:75:LYS:HB3	1.59	0.84
1:D:110:ILE:HB	1:D:113:SER:HB3	1.60	0.83

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	387/389 (100%)	369 (95%)	15 (4%)	3 (1%)	19 13
1	B	387/389 (100%)	369 (95%)	14 (4%)	4 (1%)	15 9
1	C	387/389 (100%)	372 (96%)	12 (3%)	3 (1%)	19 13
1	D	387/389 (100%)	371 (96%)	14 (4%)	2 (0%)	29 23
All	All	1548/1556 (100%)	1481 (96%)	55 (4%)	12 (1%)	19 13

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	B	72	THR
1	B	169	SER
1	B	223	ASP
1	C	223	ASP

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 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	331/331 (100%)	324 (98%)	7 (2%)	53	57
1	B	331/331 (100%)	323 (98%)	8 (2%)	49	51
1	C	331/331 (100%)	325 (98%)	6 (2%)	59	63
1	D	331/331 (100%)	324 (98%)	7 (2%)	53	57
All	All	1324/1324 (100%)	1296 (98%)	28 (2%)	53	57

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	267	LEU
1	D	234	LEU
1	C	197	TRP
1	D	149	LEU
1	C	162	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	28	ASN
1	D	111	ASN
1	D	209	ASN
1	B	92	ASN
1	B	73	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 monosaccharides 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.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.