Full wwPDB X-ray Structure Validation Report (i)

Mar 13, 2018 – 11:18 pm GMT

PDB ID	:	2VNM
Title	:	Human BACE-1 in complex with 3-(1,1-dioxidotetrahydro-2H-1,2-thiazin- 2-yl)-5-(ethylamino)-N-((1S,2R)-2-hydroxy-1-(phenylmethyl)-3-(((3-(trifluoromethyl)phenyl)methyl)amino)propyl)benzamide
Authors	:	Charrier, N.; Clarke, B.; Cutler, L.; Demont, E.; Dingwall, C.; Dunsdon, R.; East, P.; Hawkins, J.; Howes, C.; Hussain, I.; Jeffrey, P.; Maile, G.; Matico, R.; Mosley, J.; Naylor, A.; OBrien, A.; Redshaw, S.; Rowland, P.; Soleil, V.; Smith, K.J.; Sweitzer, S.; Theobald, P.; Vesey, D.; Walter, D.S.; Wayne, G.
Deposited on	:	2008-02-05
Resolution	:	1.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see references (i)) were used in the production of this report:

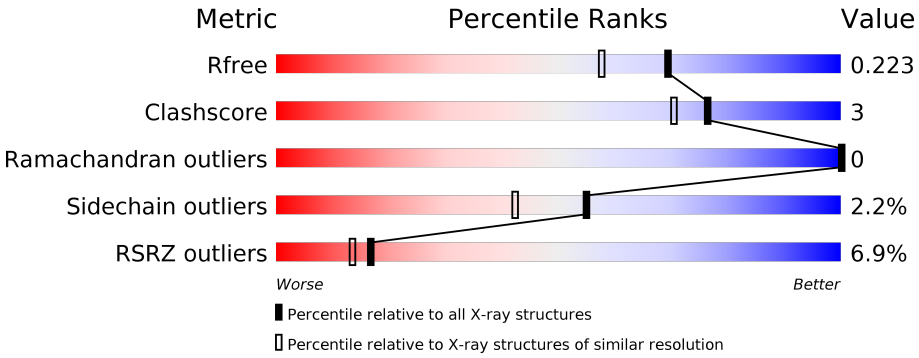
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

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 1.79 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))
R_{free}	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (1.80-1.80)

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 <=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.

Mol	Chain	Length	Quality of chain
1	A	392	7% 87% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3443 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.

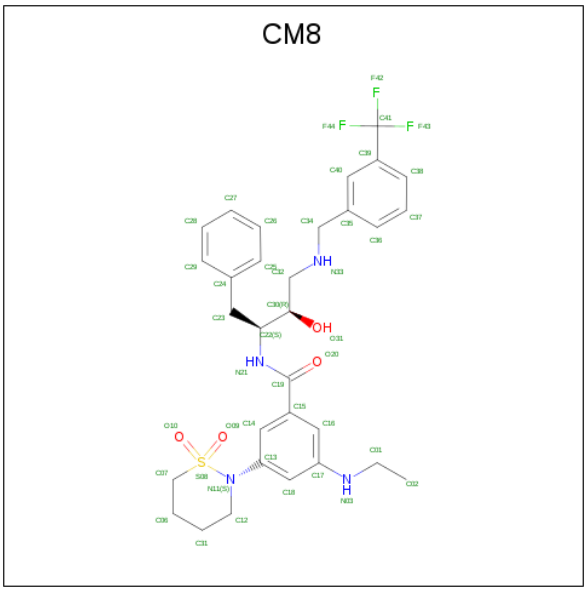
- Molecule 1 is a protein called BETA-SECRETASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	375	2991	1912	498	567	14	0	7	1

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLN	ASN	engineered mutation	UNP P56817
A	172	GLN	ASN	engineered mutation	UNP P56817
A	223	GLN	ASN	engineered mutation	UNP P56817
A	354	GLN	ASN	engineered mutation	UNP P56817

- Molecule 2 is N-[(1S,2R)-1-benzyl-2-hydroxy-3-{[3-(trifluoromethyl)benzyl]amino}propyl]-3-(1,1-dioxido-1,2-thiazinan-2-yl)-5-(ethylamino)benzamide (three-letter code: CM8) (formula: $C_{31}H_{37}F_3N_4O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			43	31	3	4	4	1		
2	A	1	Total	C	F	N	O	S	0	0
			43	31	3	4	4	1		

- Molecule 3 is water.

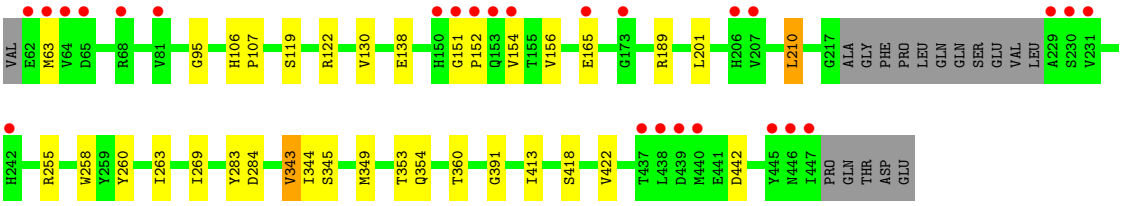
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	366	Total	O	0	0
			366	366		

3 Residue-property plots (i)

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 geometryand 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.

- Molecule 1: BETA-SECRETASE 1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	47.95Å 76.22Å 104.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.55 – 1.79 37.83 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.1 (61.55-1.79) 99.1 (37.83-1.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.3.0006	Depositor
R, R_{free}	0.191 , 0.231 0.184 , 0.223	Depositor DCC
R_{free} test set	1469 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3443	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CM8

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	0.58	0/3065	0.66	1/4167 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	LEU	CA-CB-CG	5.86	128.78	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2991	0	2897	20	0
2	A	86	0	74	1	0
3	A	366	0	0	3	0
All	All	3443	0	2971	20	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 3.

All (20) 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:152:PRO:HB2	1:A:154:VAL:HG22	1.64	0.80
1:A:349:MET:HE2	3:A:2362:HOH:O	1.91	0.69
1:A:349:MET:CE	3:A:2362:HOH:O	2.40	0.69
1:A:138:GLU:HG2	1:A:165:GLU:HB3	1.75	0.67
1:A:156:VAL:HG11	1:A:201:LEU:HA	1.83	0.59
1:A:260:TYR:HB3	1:A:413[B]:ILE:HD11	1.91	0.52
1:A:154:VAL:HG21	1:A:201:LEU:HD11	1.92	0.50
1:A:130:VAL:HG22	1:A:189:ARG:HG3	1.95	0.49
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.49	0.46
1:A:353:THR:HG22	1:A:354:GLN:HG2	1.98	0.44
1:A:119:SER:HB3	3:A:2019:HOH:O	2.17	0.43
1:A:283:TYR:O	1:A:391:GLY:HA2	2.18	0.43
1:A:345:SER:OG	1:A:360[A]:THR:HG22	2.19	0.43
1:A:269:ILE:HD12	1:A:344:ILE:HG12	2.00	0.43
1:A:95:GLY:O	2:A:2000:CM8:H40	2.19	0.42
1:A:283:TYR:HA	1:A:284:ASP:HA	1.81	0.42
1:A:269:ILE:HD13	1:A:344:ILE:HG23	2.02	0.42
1:A:63:MET:HG2	1:A:151:GLY:HA2	2.02	0.42
1:A:255:ARG:HD2	1:A:263:ILE:HD11	2.03	0.40
1:A:343:VAL:HG13	1:A:360[B]:THR:HG23	2.02	0.40

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	378/392 (96%)	371 (98%)	7 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	325/335 (97%)	318 (98%)	7 (2%)	55 42

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ARG
1	A	210	LEU
1	A	258	TRP
1	A	343	VAL
1	A	418	SER
1	A	422	VAL
1	A	442	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	272	GLN
1	A	339	ASN
1	A	355	GLN
1	A	423	HIS

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)

2 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	CM8	A	2000	-	43,46,46	2.46	22 (51%)	60,65,65	1.58	11 (18%)
2	CM8	A	2001	-	43,46,46	2.01	21 (48%)	60,65,65	1.69	5 (8%)

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	CM8	A	2000	-	-	0/35/49/49	0/4/4/4
2	CM8	A	2001	-	-	0/35/49/49	0/4/4/4

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	CM8	O20-C19	-2.64	1.17	1.23
2	A	2001	CM8	O09-S08	-2.24	1.40	1.43
2	A	2000	CM8	C14-C15	2.01	1.42	1.39
2	A	2001	CM8	C26-C25	2.03	1.42	1.38
2	A	2001	CM8	C16-C15	2.06	1.42	1.39
2	A	2000	CM8	C32-C30	2.08	1.55	1.52
2	A	2001	CM8	C28-C29	2.10	1.43	1.38
2	A	2000	CM8	O09-S08	2.18	1.45	1.43
2	A	2001	CM8	C25-C24	2.26	1.43	1.38
2	A	2001	CM8	C27-C26	2.28	1.43	1.38
2	A	2001	CM8	C41-C39	2.30	1.55	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	CM8	C28-C27	2.32	1.43	1.38
2	A	2001	CM8	C16-C17	2.44	1.43	1.39
2	A	2001	CM8	C14-C13	2.44	1.44	1.39
2	A	2000	CM8	C17-N03	2.44	1.45	1.38
2	A	2001	CM8	C40-C35	2.45	1.43	1.39
2	A	2001	CM8	C36-C35	2.46	1.44	1.38
2	A	2000	CM8	C16-C15	2.50	1.43	1.39
2	A	2001	CM8	C29-C24	2.50	1.44	1.38
2	A	2001	CM8	C37-C38	2.59	1.44	1.38
2	A	2001	CM8	C17-N03	2.60	1.46	1.38
2	A	2001	CM8	C37-C36	2.62	1.44	1.38
2	A	2000	CM8	C27-C26	2.64	1.44	1.38
2	A	2000	CM8	C37-C38	2.71	1.44	1.38
2	A	2000	CM8	C28-C29	2.86	1.44	1.38
2	A	2001	CM8	C40-C39	2.88	1.44	1.39
2	A	2000	CM8	C36-C35	3.00	1.45	1.38
2	A	2000	CM8	C40-C35	3.08	1.44	1.39
2	A	2001	CM8	C38-C39	3.12	1.44	1.39
2	A	2001	CM8	C18-C17	3.18	1.44	1.39
2	A	2000	CM8	C14-C13	3.18	1.45	1.39
2	A	2000	CM8	C37-C36	3.19	1.45	1.38
2	A	2000	CM8	C28-C27	3.20	1.45	1.38
2	A	2000	CM8	C06-C07	3.39	1.57	1.52
2	A	2000	CM8	C40-C39	3.43	1.45	1.39
2	A	2000	CM8	C26-C25	3.45	1.45	1.38
2	A	2000	CM8	C25-C24	3.59	1.46	1.38
2	A	2000	CM8	C29-C24	3.61	1.46	1.38
2	A	2000	CM8	C16-C17	3.70	1.45	1.39
2	A	2000	CM8	C38-C39	3.81	1.45	1.39
2	A	2000	CM8	C18-C17	4.60	1.47	1.39
2	A	2000	CM8	C19-N21	5.02	1.45	1.34
2	A	2001	CM8	C19-N21	5.42	1.46	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	CM8	O10-S08-O09	-9.92	108.19	118.51
2	A	2000	CM8	O10-S08-O09	-6.37	111.89	118.51
2	A	2000	CM8	C06-C07-S08	-3.15	106.61	112.19
2	A	2000	CM8	C30-C32-N33	-3.10	107.72	111.97
2	A	2000	CM8	C23-C22-N21	-3.02	106.76	110.21
2	A	2001	CM8	F42-C41-C39	-2.81	106.57	112.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	CM8	C30-C32-N33	-2.75	108.19	111.97
2	A	2000	CM8	C14-C13-N11	-2.62	114.12	119.28
2	A	2000	CM8	O31-C30-C32	-2.26	105.13	109.69
2	A	2000	CM8	F42-C41-C39	-2.25	107.84	112.94
2	A	2000	CM8	C26-C25-C24	-2.09	117.40	120.63
2	A	2000	CM8	C38-C39-C40	2.01	121.52	117.68
2	A	2000	CM8	C29-C24-C25	2.05	121.40	118.17
2	A	2001	CM8	C31-C06-C07	2.47	115.96	112.35
2	A	2000	CM8	C18-C13-N11	2.63	124.45	119.28
2	A	2001	CM8	O09-S08-C07	2.74	113.39	109.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	CM8	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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	375/392 (95%)	0.30	26 (6%)	17	13	10, 18, 32, 48	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	VAL	6.8
1	A	438	LEU	6.2
1	A	153	GLN	5.9
1	A	206	HIS	5.9
1	A	440	MET	5.5
1	A	229	ALA	5.2
1	A	62	GLU	5.0
1	A	151	GLY	4.8
1	A	446	ASN	4.6
1	A	447	ILE	4.6
1	A	152	PRO	4.1
1	A	445	TYR	3.7
1	A	437	THR	3.6
1	A	63	MET	3.4
1	A	150	HIS	3.1
1	A	65	ASP	3.0
1	A	68	ARG	3.0
1	A	154	VAL	2.8
1	A	230	SER	2.7
1	A	207	VAL	2.5
1	A	165	GLU	2.3
1	A	231	VAL	2.3
1	A	242	HIS	2.2
1	A	439	ASP	2.0
1	A	81[A]	VAL	2.0
1	A	173	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CM8	A	2001	43/43	0.89	0.15	20,20,20,20	0
2	CM8	A	2000	43/43	0.96	0.10	8,12,18,23	0

6.5 Other polymers (i)

There are no such residues in this entry.