



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 8, 2021 – 08:01 PM EDT

PDB ID : 3UQP
Title : Crystal structure of Bace1 with its inhibitor
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Deposited on : 2011-11-21
Resolution : 1.77 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

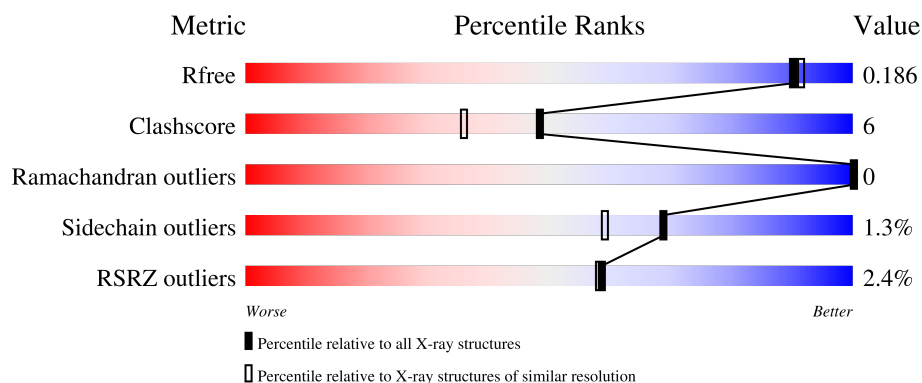
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

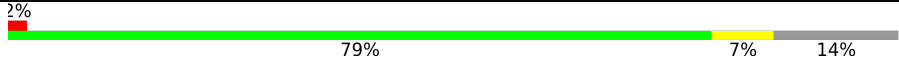

The reported resolution of this entry is 1.77 Å.

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}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	8	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PDW	B	8	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3388 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	374	2954	1892	492	556	14	0	3	0

There are 23 discrepancies between the modelled and reference sequences:

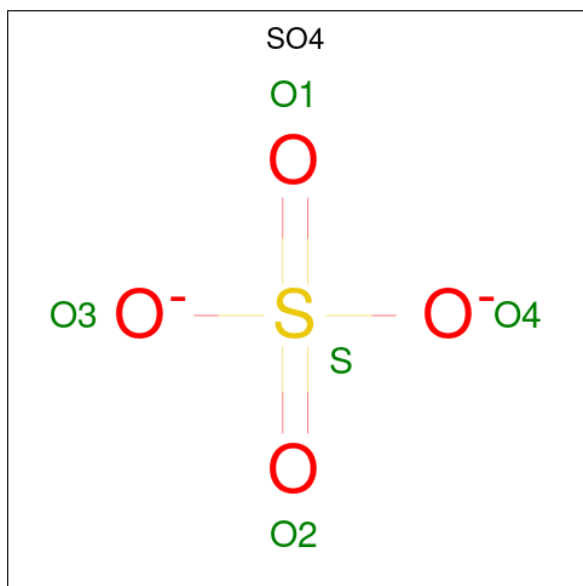
Chain	Residue	Modelled	Actual	Comment	Reference
A	9P	MET	-	expression tag	UNP P56817
A	10P	GLY	-	expression tag	UNP P56817
A	11P	SER	-	expression tag	UNP P56817
A	12P	SER	-	expression tag	UNP P56817
A	13P	HIS	-	expression tag	UNP P56817
A	14P	HIS	-	expression tag	UNP P56817
A	15P	HIS	-	expression tag	UNP P56817
A	16P	HIS	-	expression tag	UNP P56817
A	17P	HIS	-	expression tag	UNP P56817
A	18P	HIS	-	expression tag	UNP P56817
A	19P	SER	-	expression tag	UNP P56817
A	20P	ALA	-	expression tag	UNP P56817
A	21P	GLY	-	expression tag	UNP P56817
A	22P	GLU	-	expression tag	UNP P56817
A	23P	ASN	-	expression tag	UNP P56817
A	24P	LEU	-	expression tag	UNP P56817
A	25P	TYR	-	expression tag	UNP P56817
A	26P	PHE	-	expression tag	UNP P56817
A	27P	GLN	-	expression tag	UNP P56817
A	28P	GLY	-	expression tag	UNP P56817
A	29P	THR	-	expression tag	UNP P56817
A	75	ALA	LYS	engineered mutation	UNP P56817
A	77	ALA	GLU	engineered mutation	UNP P56817

- Molecule 2 is a protein called METHYL (2R)-1-[(6S,9S,12S,13S,17S,20S,23R)-9-(3-AMINO-3-OXOPROPYL)-12,23-DIBENZYL-13-HYDROXY-2,2,8,20,22-PENTAMETHYL-17-(2-METHYLPROPYL)-4,7,10,15,18,21,24-HEPTAOXO-6-(PROPAN-2-YL)-3-OXA-5,8,11,16,1

9,22-HEXAAZATETRACOSAN-24-YL]PYRROLIDINE-2-CARBOXYLATE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	8	Total	C	N	O	0	0	0
			72	52	8	12			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

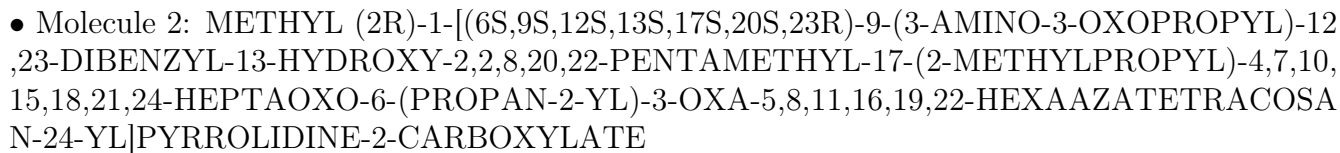


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	350	Total	O	0	0
			350	350		
4	B	2	Total	O	0	0
			2	2		

- Molecule 1: Beta-secretase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.39Å 128.06Å 76.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.46 – 1.77 40.46 – 1.77	Depositor EDS
% Data completeness (in resolution range)	87.4 (40.46-1.77) 87.4 (40.46-1.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 1.77Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.165 , 0.189 0.164 , 0.186	Depositor DCC
R_{free} test set	1312 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3388	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 6.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PDW, SO4, ZAE, GNC, BOC, PSA

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	0.35	0/3037	0.52	0/4126
2	B	1.45	1/18 (5.6%)	1.40	0/22
All	All	0.36	1/3055 (0.0%)	0.53	0/4148

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
2	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	LEU	C-N	5.58	1.46	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	4	PSA	Mainchain,Peptide

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	2954	0	2868	31	0
2	B	72	0	78	11	0
3	A	10	0	0	0	0
4	A	350	0	0	4	0
4	B	2	0	0	0	0
All	All	3388	0	2946	36	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 6.

The worst 5 of 36 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:310:GLU:HA	1:A:311:ASP:CB	2.05	0.85
1:A:310:GLU:HA	1:A:311:ASP:HB2	1.77	0.65
1:A:126:ILE:HB	2:B:8:PDW:HB2	1.80	0.62
1:A:310:GLU:HA	1:A:311:ASP:CG	2.18	0.62
1:A:232:THR:HB	2:B:1:BOC:H33	1.83	0.61

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	371/433 (86%)	366 (99%)	5 (1%)	0	100	100
2	B	3/8 (38%)	3 (100%)	0	0	100	100
All	All	374/441 (85%)	369 (99%)	5 (1%)	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	320/368 (87%)	316 (99%)	4 (1%)	69	59
2	B	2/2 (100%)	2 (100%)	0	100	100
All	All	322/370 (87%)	318 (99%)	4 (1%)	69	62

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	TRP
1	A	271	GLN
1	A	307	ARG
1	A	311	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	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](#)

4 non-standard protein/DNA/RNA residues 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	PSA	B	4	2	14,14,15	3.70	8 (57%)	15,17,19	2.10	4 (26%)
2	ZAE	B	7	2	11,12,13	4.21	6 (54%)	13,14,16	1.81	3 (23%)
2	PDW	B	8	2	9,9,9	1.27	1 (11%)	11,11,11	2.26	5 (45%)
2	GNC	B	3	2	8,9,10	1.27	1 (12%)	7,10,12	1.31	1 (14%)

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	PSA	B	4	2	-	4/11/11/12	0/1/1/1
2	ZAE	B	7	2	-	1/5/8/10	0/1/1/1
2	PDW	B	8	2	-	5/6/13/13	0/1/1/1
2	GNC	B	3	2	-	1/6/9/11	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	ZAE	CE1-CD1	6.15	1.51	1.38
2	B	7	ZAE	CD1-CG	6.14	1.52	1.38
2	B	7	ZAE	CE2-CD2	6.10	1.51	1.38
2	B	4	PSA	CE2-CD2	6.03	1.51	1.38
2	B	4	PSA	CD2-CG	5.81	1.51	1.38

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	ZAE	CG-CB-CA	-4.82	106.73	113.63
2	B	4	PSA	OH-CH-CA	4.59	117.69	109.40
2	B	4	PSA	OH-CH-CM	4.41	118.55	109.08
2	B	8	PDW	C-CA-N	4.27	118.85	111.08
2	B	8	PDW	CB-CA-C	-3.44	104.42	113.01

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	PSA	OH-CH-CM-C
2	B	4	PSA	O-C-CM-CH

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Mol	Chain	Res	Type	Atoms
2	B	8	PDW	OXT-C-CA-N
2	B	8	PDW	CA-C-OXT-CM
2	B	8	PDW	OXT-C-CA-CB

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	7	ZAE	1	0
2	B	8	PDW	6	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	$\# Z > 2$
3	SO4	A	501	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	A	502	-	4,4,4	0.21	0	6,6,6	0.25	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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, 95th 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	374/433 (86%)	-0.35	9 (2%) 59 58	10, 16, 37, 71	0
2	B	3/8 (37%)	0.05	0 100 100	22, 22, 27, 35	0
All	All	377/441 (85%)	-0.34	9 (2%) 59 58	10, 16, 37, 71	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	ASP	5.6
1	A	310	GLU	4.0
1	A	365	PHE	3.4
1	A	49	HIS	3.1
1	A	316	GLN	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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	PDW	B	8	9/9	0.73	0.31	37,42,53,54	0
2	ZAE	B	7	12/13	0.78	0.19	30,49,55,58	0
2	GNC	B	3	10/11	0.91	0.13	20,26,37,41	0
2	PSA	B	4	14/15	0.95	0.08	16,22,27,27	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95th 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
3	SO4	A	501	5/5	0.93	0.23	34,42,51,52	0
3	SO4	A	502	5/5	0.98	0.07	18,22,24,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.