wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2020 – 11:56 pm BST

PDB ID	:	5MCQ
Title	:	CRYSTAL STRUCTURE OF BACE-1 IN COMPLEX WITH ACTIVE SITE AND EXOSITE BINDING PEPTIDE INHIBITOR
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Deposited on	:	2016-11-10
Resolution	:	1.82 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 following versions of software and data (see references (1)) were used in the production of this report:

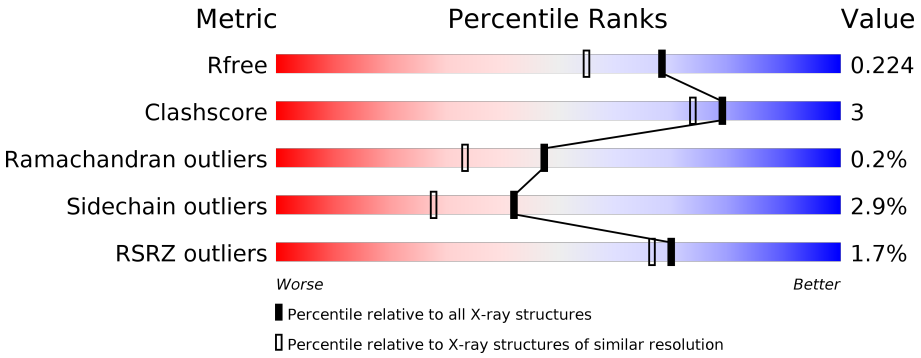
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

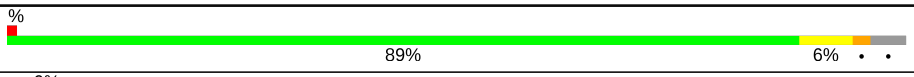
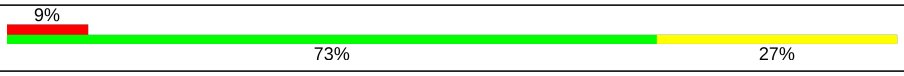
The reported resolution of this entry is 1.82 Å.

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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 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% 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	409	
2	D	22	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3887 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.

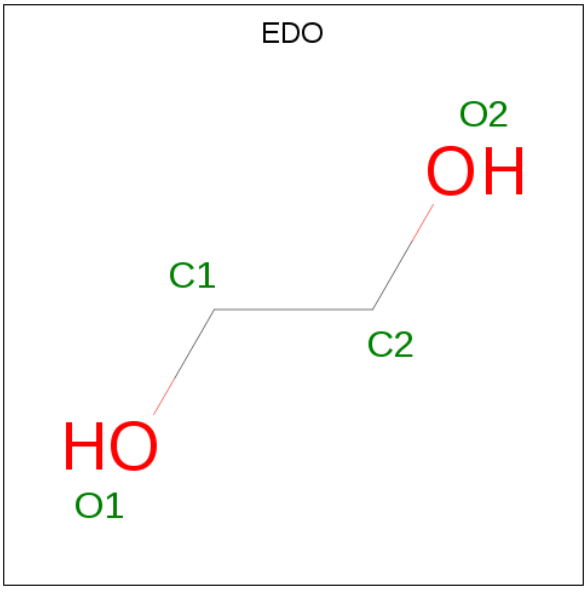
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	5	0
			3118	1997	520	587	14			

- Molecule 2 is a protein called BACE-1 ACTIVE AND EXOSITE BINDING INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	22	Total	C	N	O	0	2	1
			167	109	27	31			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

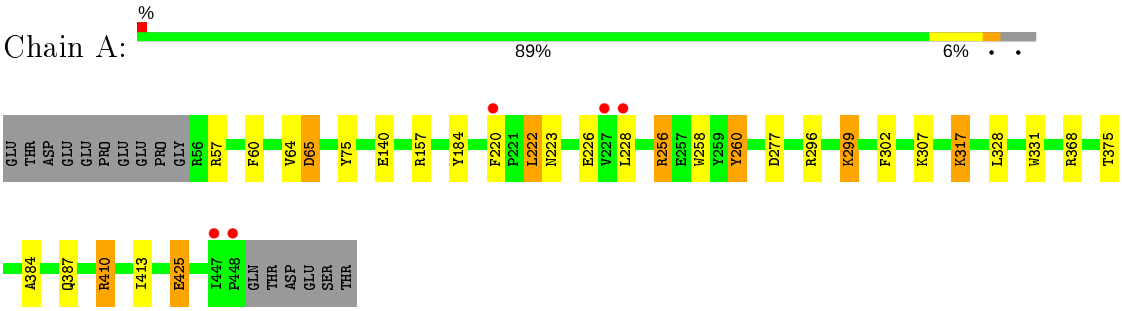
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	551	Total O 551 551	0	0
4	D	35	Total O 35 35	0	0

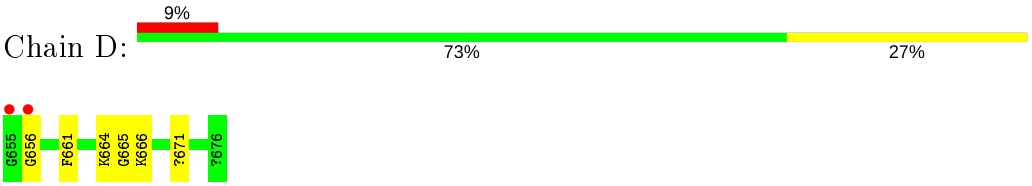
3 Residue-property plots (i)

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 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.

- Molecule 1: Beta-secretase 1



- Molecule 2: BACE-1 ACTIVE AND EXOSITE BINDING INHIBITOR



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	101.93Å 101.93Å 116.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.58 – 1.82 48.58 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.58-1.82) 99.9 (48.58-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.178 , 0.224 0.178 , 0.224	Depositor DCC
R_{free} test set	3169 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3887	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: DPR, DLY, NH2, STA, EDO

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	1.00	4/3209 (0.1%)	0.98	9/4363 (0.2%)
2	D	1.10	0/131	0.83	0/172
All	All	1.01	4/3340 (0.1%)	0.98	9/4535 (0.2%)

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	D	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	TYR	CG-CD2	5.73	1.46	1.39
1	A	75	TYR	CE1-CZ	5.60	1.45	1.38
1	A	260	TYR	CE1-CZ	5.21	1.45	1.38
1	A	331	TRP	CE3-CZ3	5.13	1.47	1.38

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	296	ARG	NE-CZ-NH2	11.14	125.87	120.30
1	A	256	ARG	NE-CZ-NH2	-9.41	115.60	120.30
1	A	296	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	A	157	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	157	ARG	NE-CZ-NH1	6.81	123.70	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	665	GLY	Peptide
2	D	671	STA	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	3118	0	3042	15	0
2	D	167	0	153	3	0
3	A	16	0	24	2	0
4	A	551	0	0	4	1
4	D	35	0	0	2	0
All	All	3887	0	3219	18	1

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.

The worst 5 of 18 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)
2:D:666:DLY:HB2	4:D:707:HOH:O	1.79	0.82
3:A:502:EDO:H12	4:A:1005:HOH:O	1.78	0.82
1:A:140:GLU:HG2	4:A:971:HOH:O	1.90	0.71
1:A:299:LYS:HG3	1:A:387[A]:GLN:CD	2.17	0.64
1:A:425:GLU:H	1:A:425:GLU:CD	2.02	0.63

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1127:HOH:O	4:A:1127:HOH:O[5_554]	1.51	0.69

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	396/409 (97%)	390 (98%)	6 (2%)	0	100 100
2	D	17/22 (77%)	14 (82%)	1 (6%)	2 (12%)	0 0
All	All	413/431 (96%)	404 (98%)	7 (2%)	2 (0%)	47 15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	656[A]	GLY
2	D	656[B]	GLY

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	340/350 (97%)	330 (97%)	10 (3%)	42 28
2	D	11/11 (100%)	11 (100%)	0	100 100
All	All	351/361 (97%)	341 (97%)	10 (3%)	42 29

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	TRP
1	A	299	LYS
1	A	375	THR
1	A	228	LEU

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Mol	Chain	Res	Type
1	A	317	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	A	423	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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	STA	D	671	2	10,10,11	1.49	2 (20%)	9,12,14	1.56	2 (22%)

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	STA	D	671	2	-	2/11/11/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	671	STA	OH-CH	2.42	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	671	STA	CH-CA	2.21	1.55	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	671	STA	O-C-CM	-3.35	115.66	125.43
2	D	671	STA	CM-CH-CA	2.22	116.43	112.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	671	STA	O-C-CM-CH
2	D	671	STA	OH-CH-CM-C

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	EDO	A	503	-	3,3,3	0.30	0	2,2,2	0.70	0
3	EDO	A	502	-	3,3,3	0.35	0	2,2,2	0.68	0
3	EDO	A	504	-	3,3,3	0.47	0	2,2,2	0.45	0
3	EDO	A	501	-	3,3,3	0.40	0	2,2,2	0.41	0

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
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	A	501	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	EDO	O1-C1-C2-O2
3	A	501	EDO	O1-C1-C2-O2
3	A	504	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	EDO	2	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	393/409 (96%)	-0.64	5 (1%) 77 74	17, 26, 54, 107	7 (1%)
2	D	17/22 (77%)	0.34	2 (11%) 4 3	18, 33, 61, 69	0
All	All	410/431 (95%)	-0.60	7 (1%) 70 66	17, 27, 54, 107	7 (1%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	656[A]	GLY	6.1
1	A	228	LEU	4.0
2	D	655[A]	GLY	3.7
1	A	447	ILE	3.3
1	A	227	VAL	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

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	DLY	D	666	9/10	0.93	0.15	46,63,73,74	0
2	DLY	D	664	9/10	0.94	0.22	52,61,90,91	0
2	DPR	D	675	7/8	0.95	0.09	40,47,53,56	0
2	STA	D	671	11/12	0.99	0.11	16,18,20,20	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
3	EDO	A	504	4/4	0.51	0.34	81,87,91,92	0
3	EDO	A	502	4/4	0.92	0.09	40,41,42,50	0
3	EDO	A	503	4/4	0.95	0.15	42,45,48,59	0
3	EDO	A	501	4/4	0.98	0.08	42,44,45,47	0

6.5 Other polymers

There are no such residues in this entry.