



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 09:00 pm GMT

PDB ID : 1BIM
Title : CRYSTALLOGRAPHIC STUDIES ON THE BINDING MODES OF P2-P3
BUTANEDIAMIDE RENIN INHIBITORS
Authors : Tong, L.
Deposited on : 1995-09-27
Resolution : 2.80 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

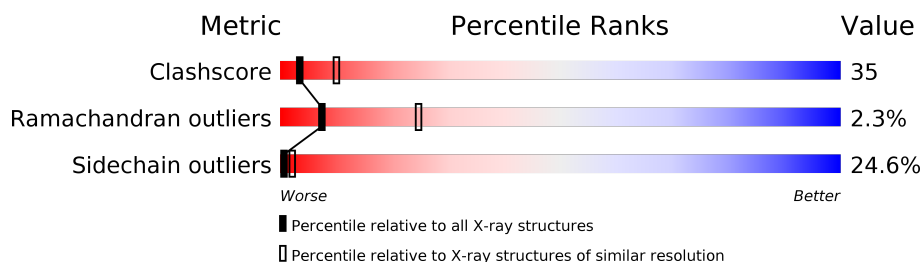
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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 $\leq 5\%$. 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	337	 34% 45% 18% ..
1	B	337	 34% 46% 18% ..

2 Entry composition [i](#)

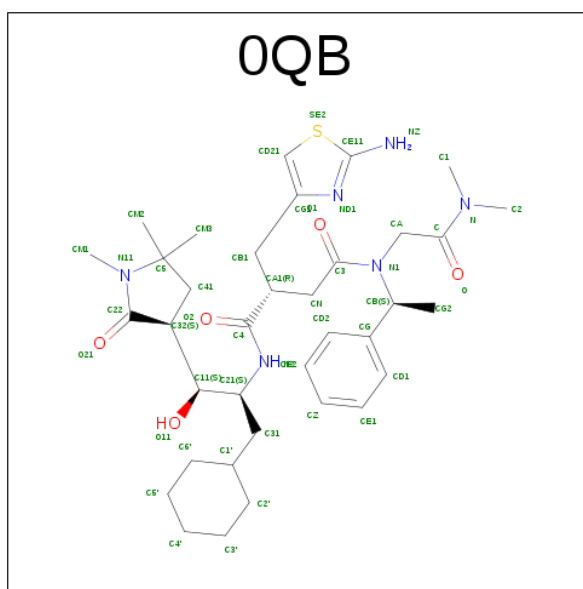
There are 2 unique types of molecules in this entry. The entry contains 5221 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Renin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2575	1644	416	501	14			
1	B	333	Total	C	N	O	S	0	0	0
			2550	1630	408	498	14			

- Molecule 2 is (2S)-2-[(2-AMINO-1,3-THIAZOL-4-YL)METHYL]-N 1 -{(1S,2S)-1-(CYCLOHEXYLMETHYL)-2-HYDROXY-2-[(3R)-1,5,5-TRIMETHYL-2-OXOPYRROLIDIN-3-YL]ETHYL}-N 4 -[2-(DIMETHYLAMINO)-2-OXOETHYL]-N 4 -[(1S)-1-PHENYLETHYL]BUTANEDIAMIDE (three-letter code: 0QB) (formula: C₃₆H₅₄N₆O₅S).

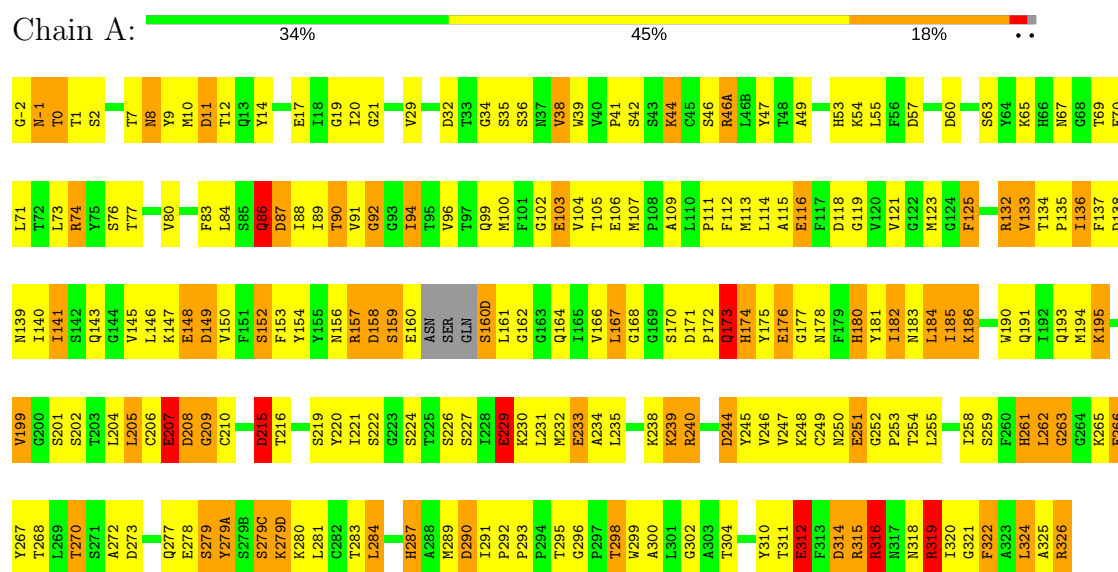


3 Residue-property plots

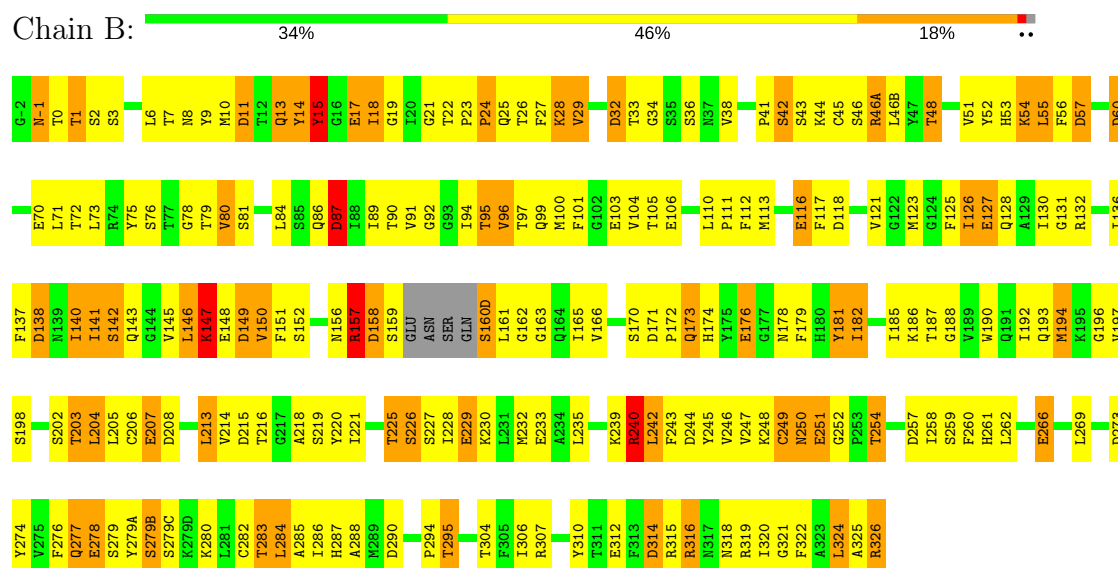
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Renin



• Molecule 1: Renin



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	142.90Å 142.90Å 142.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5221	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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: 0QB

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	1.12	15/2634 (0.6%)	1.59	42/3570 (1.2%)
1	B	1.12	14/2609 (0.5%)	1.56	39/3540 (1.1%)
All	All	1.12	29/5243 (0.6%)	1.57	81/7110 (1.1%)

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
1	A	1	0
1	B	1	0
All	All	2	0

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	148	GLU	CD-OE1	10.04	1.36	1.25
1	B	229	GLU	CD-OE1	9.12	1.35	1.25
1	A	148	GLU	CD-OE2	9.06	1.35	1.25
1	B	278	GLU	CD-OE2	9.00	1.35	1.25
1	A	251	GLU	CD-OE2	8.86	1.35	1.25

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	ASP	CB-CG-OD2	-11.55	107.90	118.30
1	A	314	ASP	CB-CG-OD1	11.41	128.57	118.30
1	A	60	ASP	CB-CG-OD2	-9.63	109.63	118.30
1	B	149	ASP	CB-CG-OD1	-9.60	109.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ARG	NE-CZ-NH2	-9.15	115.72	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	215	ASP	CA
1	B	112	PHE	CA

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	2575	0	2507	174	0
1	B	2550	0	2468	168	0
2	A	48	0	54	18	0
2	B	48	0	54	17	0
All	All	5221	0	5083	363	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 35.

The worst 5 of 363 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:A:391:0QB:HD21	2:A:391:0QB:CD21	0.97	1.09
1:A:195:LYS:HB2	1:A:261:HIS:HD2	1.11	1.06
2:B:391:0QB:CD21	2:B:391:0QB:HD21	0.97	1.05
2:B:391:0QB:SE2	2:B:391:0QB:CG1	2.55	1.04
2:B:391:0QB:CD21	2:B:391:0QB:SE2	1.78	1.03

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	330/337 (98%)	288 (87%)	33 (10%)	9 (3%)	6	20
1	B	329/337 (98%)	284 (86%)	39 (12%)	6 (2%)	10	32
All	All	659/674 (98%)	572 (87%)	72 (11%)	15 (2%)	7	25

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ILE
1	A	316	ARG
1	B	112	PHE
1	B	242	LEU
1	A	92	GLY

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	284/287 (99%)	213 (75%)	71 (25%)	1	2
1	B	280/287 (98%)	212 (76%)	68 (24%)	1	2
All	All	564/574 (98%)	425 (75%)	139 (25%)	1	2

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	312	GLU

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Mol	Chain	Res	Type
1	B	24	PRO
1	B	240	ARG
1	A	316	ARG
1	A	326	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	193	GLN
1	B	139	ASN
1	A	173	GLN
1	A	174	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	0QB	A	391	-	47,51,51	2.03	16 (34%)	51,73,73	2.12	14 (27%)
2	0QB	B	391	-	47,51,51	1.77	11 (23%)	51,73,73	2.21	10 (19%)

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	0QB	A	391	-	-	0/47/75/75	0/4/4/4
2	0QB	B	391	-	-	0/47/75/75	0/4/4/4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	391	0QB	C5-N11	-5.15	1.42	1.48
2	B	391	0QB	C5-N11	-3.66	1.44	1.48
2	A	391	0QB	CD2-CG	-2.99	1.34	1.39
2	A	391	0QB	CD1-CG	-2.95	1.34	1.39
2	B	391	0QB	CE1-CD1	-2.85	1.33	1.38

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	391	0QB	CG2-CB-CG	-9.90	88.83	113.18
2	A	391	0QB	O2-C4-CA1	-5.33	115.28	122.11
2	A	391	0QB	CB1-CG1-CD21	-4.78	121.50	130.18
2	B	391	0QB	CB1-CG1-CD21	-4.53	121.95	130.18
2	A	391	0QB	CG2-CB-N1	-4.37	105.61	110.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	391	0QB	18	0
2	B	391	0QB	17	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.