



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 06:56 pm BST

PDB ID : 1GNV  
Title : CALCIUM INDEPENDENT SUBTILISIN BPN' MUTANT  
Authors : Almog, O.; Gilliland, G.L.  
Deposited on : 2001-10-10  
Resolution : 1.90 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](mailto: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.

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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) : **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) : 2.11

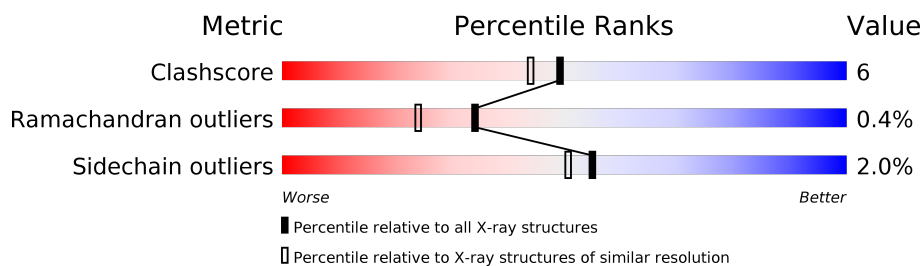
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	266	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2014 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 SUBTILISIN BPN'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	P	S	0	1	0
			1881	1167	322	385	1	6			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LYS	GLU	engineered mutation	UNP P00782
A	3	CYS	SER	engineered mutation	UNP P00782
A	5	SER	PRO	engineered mutation	UNP P00782
A	43	ASN	LYS	engineered mutation	UNP P00782
A	50	PHE	MET	engineered mutation	UNP P00782
A	73	LEU	ALA	engineered mutation	UNP P00782
A	206	CYS	GLU	engineered mutation	UNP P00782
A	217	LYS	TYR	engineered mutation	UNP P00782
A	218	SER	ASN	engineered mutation	UNP P00782
A	221	MIS	SER	engineered mutation	UNP P00782
A	271	GLU	GLN	engineered mutation	UNP P00782

- Molecule 2 is water.

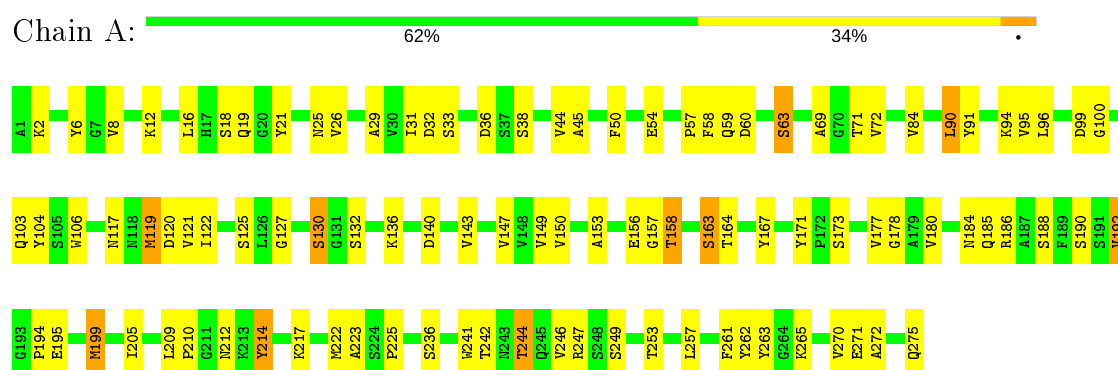
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	133	Total	O	0	0
			133	133		

### 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. 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: SUBTILISIN BPN'



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.20 Å 60.40 Å 82.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.90	Depositor
% Data completeness (in resolution range)	86.0 (8.00-1.90)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2014	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	1.51	4/1909 (0.2%)	2.37	94/2602 (3.6%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	SER	CB-OG	-6.70	1.33	1.42
1	A	157	GLY	CA-C	5.47	1.60	1.51
1	A	72	VAL	CB-CG1	5.27	1.64	1.52
1	A	190	SER	CA-CB	5.26	1.60	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ARG	NE-CZ-NH2	-21.36	109.62	120.30
1	A	104	TYR	CB-CG-CD1	14.40	129.64	121.00
1	A	50	PHE	CB-CG-CD2	-13.18	111.58	120.80
1	A	50	PHE	CB-CG-CD1	12.10	129.27	120.80
1	A	244	THR	CA-CB-CG2	10.47	127.06	112.40
1	A	261	PHE	CB-CG-CD1	-9.34	114.26	120.80
1	A	186	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A	186	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	A	91	TYR	CB-CG-CD2	8.87	126.32	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	THR	CA-CB-CG2	8.62	124.47	112.40
1	A	63	SER	N-CA-CB	8.61	123.41	110.50
1	A	186	ARG	CD-NE-CZ	8.26	135.16	123.60
1	A	244	THR	OG1-CB-CG2	8.24	128.95	110.00
1	A	192	VAL	CA-CB-CG2	8.11	123.07	110.90
1	A	272	ALA	CB-CA-C	7.92	121.98	110.10
1	A	262	TYR	CB-CG-CD1	7.81	125.69	121.00
1	A	257	LEU	CA-C-N	7.53	131.25	116.20
1	A	262	TYR	CB-CG-CD2	-7.50	116.50	121.00
1	A	185	GLN	CB-CG-CD	7.33	130.65	111.60
1	A	247	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	140	ASP	CB-CG-OD1	7.04	124.63	118.30
1	A	104	TYR	CA-CB-CG	6.99	126.68	113.40
1	A	104	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	A	99	ASP	CB-CG-OD1	6.88	124.50	118.30
1	A	158	THR	CA-CB-CG2	6.78	121.89	112.40
1	A	58	PHE	CB-CG-CD1	-6.76	116.07	120.80
1	A	16	LEU	CB-CG-CD1	-6.69	99.63	111.00
1	A	54	GLU	CA-CB-CG	6.69	128.11	113.40
1	A	247	ARG	NH1-CZ-NH2	6.49	126.54	119.40
1	A	130	SER	CB-CA-C	6.47	122.40	110.10
1	A	188	SER	CB-CA-C	6.47	122.39	110.10
1	A	32	ASP	CB-CG-OD2	6.44	124.10	118.30
1	A	177	VAL	CA-CB-CG2	6.40	120.50	110.90
1	A	275	GLN	CB-CA-C	6.31	123.02	110.40
1	A	253	THR	O-C-N	-6.20	112.78	122.70
1	A	84	VAL	CG1-CB-CG2	-6.12	101.12	110.90
1	A	45	ALA	O-C-N	-6.11	112.81	123.20
1	A	195	GLU	C-N-CA	6.08	136.89	121.70
1	A	164	THR	CA-CB-CG2	6.07	120.90	112.40
1	A	19	GLN	O-C-N	-6.03	112.95	123.20
1	A	44	VAL	CG1-CB-CG2	-6.02	101.27	110.90
1	A	212	ASN	CB-CA-C	6.01	122.41	110.40
1	A	199	MET	CA-CB-CG	5.99	123.48	113.30
1	A	95	VAL	CA-CB-CG2	5.99	119.88	110.90
1	A	59	GLN	CB-CG-CD	5.95	127.08	111.60
1	A	57	PRO	C-N-CA	5.87	136.37	121.70
1	A	25	ASN	CB-CG-OD1	-5.84	109.91	121.60
1	A	90	LEU	CA-CB-CG	5.83	128.70	115.30
1	A	100	GLY	C-N-CA	5.79	136.18	121.70
1	A	18	SER	CB-CA-C	5.74	121.01	110.10
1	A	21	TYR	CB-CG-CD1	5.74	124.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	117	ASN	O-C-N	-5.66	113.65	122.70
1	A	265	LYS	O-C-N	-5.66	113.58	123.20
1	A	26	VAL	C-N-CA	5.65	135.83	121.70
1	A	21	TYR	CB-CA-C	5.63	121.66	110.40
1	A	104	TYR	CG-CD1-CE1	5.63	125.80	121.30
1	A	33	SER	C-N-CA	5.61	134.09	122.30
1	A	6	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	A	121	VAL	CA-CB-CG2	5.53	119.19	110.90
1	A	271	GLU	CG-CD-OE1	5.49	129.29	118.30
1	A	150	VAL	CA-CB-CG2	5.48	119.12	110.90
1	A	120	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	241	TRP	CB-CG-CD1	5.48	134.12	127.00
1	A	21	TYR	CZ-CE2-CD2	-5.46	114.88	119.80
1	A	119	MET	CA-CB-CG	5.45	122.56	113.30
1	A	270	VAL	CB-CA-C	5.45	121.75	111.40
1	A	214	TYR	CB-CG-CD1	5.41	124.25	121.00
1	A	163[A]	SER	N-CA-CB	5.40	118.60	110.50
1	A	163[B]	SER	N-CA-CB	5.40	118.60	110.50
1	A	33	SER	O-C-N	-5.40	114.02	123.20
1	A	271	GLU	CG-CD-OE2	-5.40	107.51	118.30
1	A	95	VAL	CA-CB-CG1	5.36	118.94	110.90
1	A	8	VAL	CA-CB-CG1	5.34	118.92	110.90
1	A	6	TYR	CB-CG-CD1	5.33	124.19	121.00
1	A	149	VAL	CA-CB-CG2	5.32	118.88	110.90
1	A	257	LEU	O-C-N	-5.32	114.15	123.20
1	A	214	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	184	ASN	O-C-N	-5.31	114.21	122.70
1	A	246	VAL	CA-CB-CG1	5.29	118.83	110.90
1	A	178	GLY	O-C-N	-5.27	114.27	122.70
1	A	58	PHE	CB-CG-CD2	5.26	124.48	120.80
1	A	125	SER	C-N-CA	5.25	134.84	121.70
1	A	180	VAL	CA-CB-CG2	5.25	118.78	110.90
1	A	153	ALA	C-N-CA	5.25	133.33	122.30
1	A	106	TRP	CA-CB-CG	5.24	123.66	113.70
1	A	156	GLU	O-C-N	-5.22	114.33	123.20
1	A	184	ASN	CA-C-O	5.20	131.01	120.10
1	A	205	ILE	CA-CB-CG2	5.18	121.25	110.90
1	A	12	LYS	O-C-N	-5.17	114.44	122.70
1	A	241	TRP	CA-CB-CG	5.16	123.50	113.70
1	A	60	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	94	LYS	CA-C-O	5.01	130.63	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ALA	CB-CA-C	5.01	117.61	110.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	244	THR	CB

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	1881	0	1838	22	0
2	A	133	0	0	5	0
All	All	2014	0	1838	22	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.

All (22) 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:31:ILE:HD12	1:A:122:ILE:HG23	1.77	0.66
1:A:69:ALA:HB1	1:A:90:LEU:HD21	1.81	0.62
1:A:136:LYS:HG3	1:A:171:TYR:CD1	2.37	0.60
1:A:103:GLN:HG3	2:A:2057:HOH:O	2.04	0.58
1:A:2:LYS:HG3	1:A:214:TYR:CZ	2.39	0.57
1:A:31:ILE:HD12	1:A:122:ILE:CG2	2.35	0.56
1:A:143:VAL:HG21	1:A:173:SER:HB2	1.87	0.55
1:A:199:MET:HG2	1:A:263:TYR:O	2.06	0.55
1:A:236:SER:HA	2:A:2019:HOH:O	2.07	0.55
1:A:163[A]:SER:HB2	1:A:194:PRO:HD2	1.92	0.51
1:A:158:THR:HG22	1:A:192:VAL:HG21	1.93	0.51
1:A:163[B]:SER:HB3	1:A:194:PRO:HD2	1.92	0.50
1:A:158:THR:HB	2:A:2088:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:THR:HG21	1:A:225:PRO:HG2	1.97	0.45
1:A:29:ALA:HB2	1:A:119:MET:HG3	1.99	0.45
1:A:122:ILE:HD12	1:A:147:VAL:HG11	1.99	0.44
1:A:2:LYS:N	2:A:2001:HOH:O	2.51	0.43
1:A:209:LEU:HD21	1:A:217:LYS:HE2	2.00	0.43
1:A:36:ASP:OD2	1:A:210:PRO:HA	2.20	0.42
1:A:127:GLY:HA2	1:A:167:TYR:O	2.20	0.41
1:A:130:SER:HB3	2:A:2068:HOH:O	2.21	0.41
1:A:31:ILE:CD1	1:A:122:ILE:HG23	2.49	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	264/266 (99%)	259 (98%)	4 (2%)	1 (0%)	34 24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	SER

### 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	199/198 (100%)	195 (98%)	4 (2%)	55 51

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

Mol	Chain	Res	Type
1	A	38	SER
1	A	222	MET
1	A	244	THR
1	A	249	SER

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

Mol	Chain	Res	Type
1	A	275	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	MIS	A	221	1	11,12,13	1.94	4 (36%)	10,16,18	1.56	3 (30%)

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
1	MIS	A	221	1	-	2/10/13/15	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	MIS	P-O1P	-3.59	1.38	1.55
1	A	221	MIS	P-O2P	-3.15	1.39	1.50
1	A	221	MIS	P-O3P	2.84	1.68	1.60
1	A	221	MIS	C3-C1	2.24	1.61	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	MIS	O3P-C1-C3	-2.55	98.74	107.69
1	A	221	MIS	O3P-C1-C2	2.55	116.62	107.69
1	A	221	MIS	OG-P-O2P	2.06	117.10	109.07

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	221	MIS	CA-CB-OG-P
1	A	221	MIS	CB-OG-P-O3P

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](#)

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 ⓘ

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.