



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 11:15 PM EDT

PDB ID : 3CNQ  
Title : Prosubtilisin Substrate Complex of Subtilisin SUBT\_BACAM  
Authors : Gallagher, D.T.; Bryan, P.N.  
Deposited on : unknown  
Resolution : 1.71 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

<http://wwpdb.org/validation/2016/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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

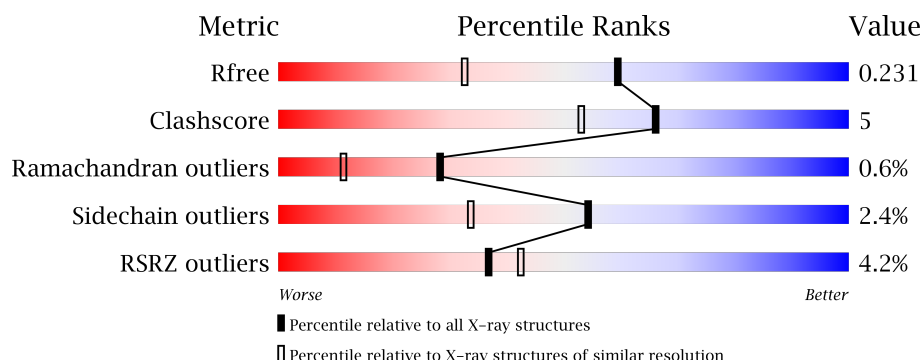
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.71 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))
$R_{free}$	100719	4385 (1.74-1.70)
Clashscore	112137	4841 (1.74-1.70)
Ramachandran outliers	110173	4771 (1.74-1.70)
Sidechain outliers	110143	4771 (1.74-1.70)
RSRZ outliers	101464	4426 (1.74-1.70)

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. 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	P	80	<div> <div>8%</div> <div>84%</div> <div>5%</div> <div>11%</div> </div>
2	S	266	<div> <div>3%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>

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
3	ZN	S	278	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2665 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
			Total	C	N	O	S			
1	P	71	558	357	91	108	2	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	2	MET	-	EXPRESSION TAG	UNP P00782
P	3	GLY	-	EXPRESSION TAG	UNP P00782
P	?	-	THR	SEE REMARK 999	UNP P00782
P	?	-	MET	SEE REMARK 999	UNP P00782
P	?	-	SER	SEE REMARK 999	UNP P00782
P	?	-	THR	SEE REMARK 999	UNP P00782
P	?	-	MET	SEE REMARK 999	UNP P00782
P	?	-	SER	SEE REMARK 999	UNP P00782
P	?	-	ALA	SEE REMARK 999	UNP P00782
P	27	GLU	LYS	ENGINEERED	UNP P00782
P	37	LEU	VAL	ENGINEERED	UNP P00782
P	40	CYS	GLN	ENGINEERED	UNP P00782
P	57	GLU	LYS	ENGINEERED	UNP P00782
P	72	LYS	HIS	ENGINEERED	UNP P00782
P	73	LEU	VAL	ENGINEERED	UNP P00782
P	74	TYR	ALA	ENGINEERED	UNP P00782
P	75	ARG	HIS	ENGINEERED	UNP P00782
P	77	LEU	TYR	ENGINEERED	UNP P00782
P	78	SER	-	EXPRESSION TAG	UNP P00782
P	79	ALA	-	EXPRESSION TAG	UNP P00782
P	80	THR	-	EXPRESSION TAG	UNP P00782
P	81	SER	-	EXPRESSION TAG	UNP P00782

- Molecule 2 is a protein called Subtilisin BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	264	Total	C	N	O	S	0	0	0
			1843	1148	317	372	6			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	2	LYS	GLN	ENGINEERED	UNP P00782
S	3	CYS	SER	ENGINEERED	UNP P00782
S	5	SER	PRO	ENGINEERED	UNP P00782
S	9	ALA	SER	ENGINEERED	UNP P00782
S	31	LEU	ILE	ENGINEERED	UNP P00782
S	32	ALA	ASP	ENGINEERED	UNP P00782
S	43	ASN	LYS	ENGINEERED	UNP P00782
S	50	PHE	MET	ENGINEERED	UNP P00782
S	?	-	VAL	DELETION	UNP P00782
S	?	-	ALA	DELETION	UNP P00782
S	?	-	ALA	DELETION	UNP P00782
S	?	-	LEU	DELETION	UNP P00782
S	?	-	ASN	DELETION	UNP P00782
S	?	-	ASN	DELETION	UNP P00782
S	?	-	SER	DELETION	UNP P00782
S	?	-	ILE	DELETION	UNP P00782
S	?	-	GLY	DELETION	UNP P00782
S	74	ALA	GLY	ENGINEERED	UNP P00782
S	104	ALA	TYR	ENGINEERED	UNP P00782
S	128	SER	GLY	ENGINEERED	UNP P00782
S	156	SER	GLU	ENGINEERED	UNP P00782
S	166	SER	GLY	ENGINEERED	UNP P00782
S	169	ALA	GLY	ENGINEERED	UNP P00782
S	188	PRO	SER	ENGINEERED	UNP P00782
S	206	CYS	GLN	ENGINEERED	UNP P00782
S	212	GLY	ASN	ENGINEERED	UNP P00782
S	217	LEU	TYR	ENGINEERED	UNP P00782
S	218	SER	ASN	ENGINEERED	UNP P00782
S	221	ALA	SER	ENGINEERED	UNP P00782
S	254	ALA	THR	ENGINEERED	UNP P00782
S	271	GLU	GLN	ENGINEERED	UNP P00782

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	5	Total	Zn	0	0
			5	5		

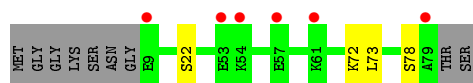
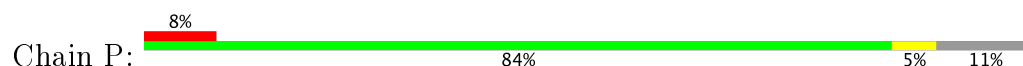
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	64	Total 64	O 64	0	0
4	S	195	Total 195	O 195	0	0

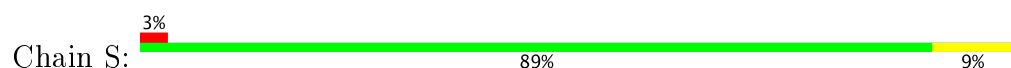
### 3 Residue-property plots [i](#)

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: Subtilisin BPN'



- Molecule 2: Subtilisin BPN'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.20Å 72.94Å 93.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.71 37.17 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.5 (10.00-1.71) 99.4 (37.17-1.71)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.69 (at 1.71Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.191 , 0.232 0.190 , 0.231	Depositor DCC
$R_{free}$ test set	1636 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2665	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	P	0.66	0/565	0.76	0/751
2	S	0.72	1/1880 (0.1%)	0.73	1/2569 (0.0%)
All	All	0.71	1/2445 (0.0%)	0.74	1/3320 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	74	ALA	C-N	5.21	1.46	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	64	HIS	CB-CA-C	5.28	120.97	110.40

There are no chirality outliers.

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	P	558	0	573	5	0
2	S	1843	0	1808	22	0
3	S	5	0	0	0	0
4	P	64	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	195	0	0	0	0
All	All	2665	0	2381	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 5.

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)
2:S:5:SER:HB3	2:S:205:ILE:HG23	1.60	0.82
1:P:72:LYS:NZ	2:S:132:SER:HB2	1.95	0.82
1:P:72:LYS:HZ2	2:S:132:SER:HB2	1.44	0.81
2:S:272:ALA:O	2:S:275:GLN:HG2	1.91	0.69
1:P:72:LYS:HE3	2:S:131:GLY:O	1.99	0.61
2:S:32:ALA:HB1	2:S:64:HIS:CE1	2.38	0.59
2:S:272:ALA:O	2:S:275:GLN:CG	2.50	0.59
2:S:13:ALA:HA	2:S:270:VAL:HG11	1.88	0.56
2:S:3:CYS:HB3	2:S:214:TYR:CD1	2.41	0.55
2:S:5:SER:C	2:S:7:GLY:H	2.10	0.53
2:S:64:HIS:CE1	2:S:96:LEU:HD12	2.44	0.53
2:S:64:HIS:HE1	2:S:96:LEU:HD12	1.74	0.52
2:S:73:LEU:HG	2:S:90:LEU:HD11	1.91	0.51
2:S:5:SER:C	2:S:7:GLY:N	2.65	0.49
2:S:39:HIS:HA	2:S:40:PRO:HD3	1.65	0.47
1:P:72:LYS:HE3	2:S:131:GLY:C	2.34	0.46
1:P:72:LYS:HZ1	2:S:132:SER:HB2	1.79	0.45
2:S:29:ALA:HB2	2:S:119:MET:HG3	1.98	0.45
2:S:62:ASN:OD1	2:S:64:HIS:HB3	2.18	0.44
2:S:13:ALA:N	2:S:14:PRO:CD	2.82	0.42
2:S:5:SER:CB	2:S:205:ILE:HG23	2.42	0.41
2:S:39:HIS:HB3	2:S:42:LEU:HB2	2.03	0.41

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	P	69/80 (86%)	68 (99%)	1 (1%)	0	100	100
2	S	262/266 (98%)	256 (98%)	4 (2%)	2 (1%)	22	7
All	All	331/346 (96%)	324 (98%)	5 (2%)	2 (1%)	28	11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	63	SER
2	S	6	TYR

### 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	P	59/65 (91%)	56 (95%)	3 (5%)	28	9
2	S	194/195 (100%)	191 (98%)	3 (2%)	70	54
All	All	253/260 (97%)	247 (98%)	6 (2%)	54	34

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	22	SER
1	P	73	LEU
1	P	78	SER
2	S	64	HIS
2	S	222	MET
2	S	275	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	S	25	ASN
2	S	59	GLN
2	S	61	ASN
2	S	64	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](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	P	71/80 (88%)	0.50	6 (8%) 11 13	14, 21, 33, 44	0
2	S	264/266 (99%)	0.12	8 (3%) 51 57	12, 17, 29, 46	0
All	All	335/346 (96%)	0.20	14 (4%) 37 42	12, 18, 32, 46	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	79	ALA	7.6
2	S	3	CYS	7.6
1	P	9	GLU	6.8
2	S	4	VAL	6.8
2	S	275	GLN	5.0
2	S	40	PRO	5.0
2	S	41	ASP	4.3
1	P	57	GLU	2.8
1	P	61	LYS	2.5
2	S	214	TYR	2.4
1	P	53	GLU	2.2
1	P	54	LYS	2.0
2	S	5	SER	2.0
2	S	185	GLN	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	S	278	1/1	0.96	0.21	10.10	39,39,39,39	0
3	ZN	S	280	1/1	0.98	0.06	-1.41	52,52,52,52	0
3	ZN	S	282	1/1	0.98	0.07	-1.50	30,30,30,30	0
3	ZN	S	279	1/1	0.98	0.05	-2.79	20,20,20,20	0
3	ZN	S	281	1/1	0.98	0.06	-	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.