



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 05:04 PM EDT

PDB ID : 2QZW  
Title : Secreted aspartic proteinase (Sap) 1 from Candida albicans  
Authors : Ruge, E.; Borelli, C.; Maskos, K.; Huber, R.  
Deposited on : unknown  
Resolution : 2.05 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

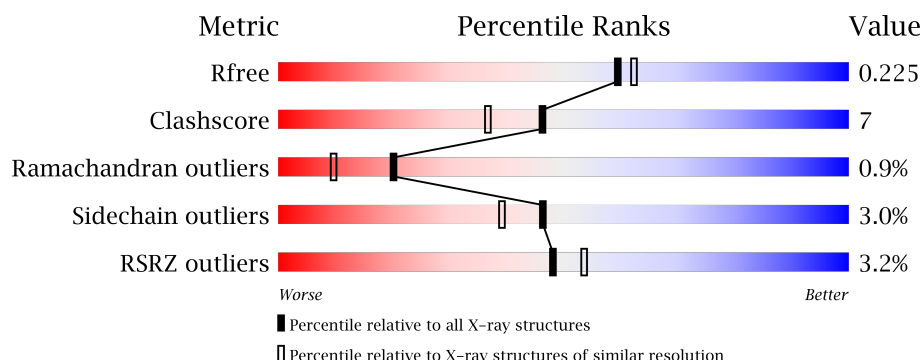
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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	A	341	<div> <div>4%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	B	341	<div> <div>3%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5763 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 Candidapepsin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	92	0	0
			2554	1607	419	524	4			
1	B	341	Total	C	N	O	S	85	0	0
			2554	1607	419	524	4			

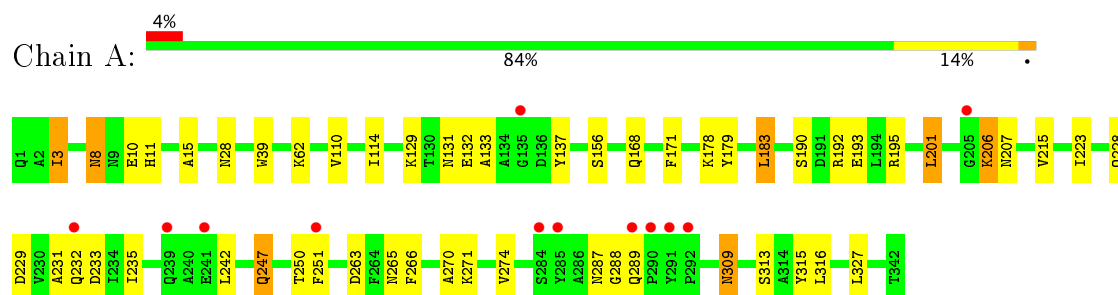
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	335	Total	O	0	0
			335	335		
2	B	320	Total	O	0	0
			320	320		

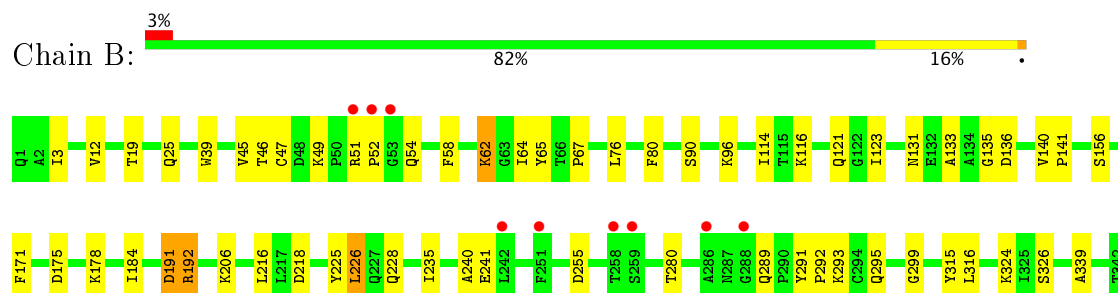
### 3 Residue-property plots [i](#)

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: Candidapepsin-1



#### • Molecule 1: Candidapepsin-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.77Å 135.67Å 96.49Å 90.00° 96.74° 90.00°	Depositor
Resolution (Å)	19.90 – 2.05 19.94 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.90-2.05) 98.0 (19.94-2.05)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	12.65 (at 2.06Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.189 , 0.224 0.191 , 0.225	Depositor DCC
$R_{free}$ test set	2382 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5763	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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

### 5.1 Standard geometry

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	0.33	0/2600	0.65	0/3539
1	B	0.33	0/2600	0.64	0/3539
All	All	0.33	0/5200	0.65	0/7078

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	2554	0	2503	32	0
1	B	2554	0	2503	39	0
2	A	335	0	0	0	0
2	B	320	0	0	4	0
All	All	5763	0	5006	70	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 7.

All (70) 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:3:ILE:HG23	1:A:171:PHE:HB2	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:CG2	1:B:171:PHE:HB2	2.00	0.90
1:A:229:ASP:O	1:A:232:GLN:HG2	1.74	0.87
1:B:324:LYS:HE3	2:B:512:HOH:O	1.77	0.83
1:A:206:LYS:HE2	1:A:207:ASN:N	2.03	0.74
1:A:206:LYS:HE2	1:A:207:ASN:H	1.53	0.74
1:A:265:ASN:HD21	1:A:271:LYS:HZ3	1.33	0.74
1:A:3:ILE:CG2	1:A:171:PHE:HB2	2.19	0.71
1:B:3:ILE:HG23	1:B:171:PHE:HB2	1.73	0.69
1:A:265:ASN:HD21	1:A:271:LYS:NZ	1.97	0.62
1:B:3:ILE:HG23	1:B:3:ILE:O	2.02	0.59
1:B:3:ILE:HG22	1:B:171:PHE:HB2	1.83	0.58
1:B:235:ILE:HG23	1:B:240:ALA:HB3	1.85	0.57
1:B:76:LEU:HD11	1:B:96:LYS:HG3	1.88	0.56
1:A:327:LEU:HD12	1:A:327:LEU:N	2.23	0.54
1:B:291:TYR:CG	1:B:292:PRO:HD2	2.42	0.54
1:A:232:GLN:HG3	1:A:233:ASP:N	2.23	0.53
1:A:156:SER:HA	1:A:316:LEU:O	2.09	0.53
1:B:123:ILE:HD11	2:B:580:HOH:O	2.09	0.52
1:B:178:LYS:HB3	1:B:315:TYR:CD1	2.45	0.52
1:A:131:ASN:OD1	1:A:192:ARG:HD2	2.09	0.52
1:B:289:GLN:HA	1:B:289:GLN:OE1	2.10	0.52
1:B:191:ASP:N	1:B:191:ASP:OD2	2.35	0.50
1:B:291:TYR:CD2	1:B:292:PRO:HD2	2.46	0.50
1:A:266:PHE:HB2	1:A:270:ALA:HB3	1.94	0.50
1:B:51:ARG:HB3	1:B:52:PRO:HD2	1.95	0.49
1:A:39:TRP:CE3	1:A:114:ILE:HG13	2.47	0.49
1:A:8:ASN:ND2	1:A:15:ALA:O	2.46	0.48
1:B:156:SER:HA	1:B:316:LEU:O	2.13	0.48
1:A:201:LEU:N	1:A:201:LEU:HD12	2.29	0.48
1:A:309:ASN:HD22	1:A:309:ASN:N	2.10	0.48
1:A:110:VAL:HB	1:A:137:TYR:CD2	2.49	0.48
1:A:179:TYR:CZ	1:A:183:LEU:HD22	2.48	0.48
1:A:274:VAL:HG22	1:A:313:SER:HB2	1.95	0.48
1:B:255:ASP:OD1	1:B:293:LYS:HE3	2.14	0.48
1:B:19:THR:HA	1:B:25:GLN:O	2.14	0.48
1:B:49:LYS:HG2	1:B:49:LYS:O	2.15	0.47
1:A:232:GLN:CG	1:A:233:ASP:N	2.77	0.47
1:A:231:ALA:O	1:A:235:ILE:HG13	2.15	0.47
1:A:8:ASN:ND2	1:A:8:ASN:H	2.12	0.47
1:B:65:TYR:CE2	1:B:67:PRO:HG3	2.50	0.46
1:B:216:LEU:HG	1:B:218:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LYS:HG2	1:B:121:GLN:NE2	2.31	0.46
1:A:10:GLU:O	1:A:11:HIS:HB2	2.16	0.45
1:B:135:GLY:O	1:B:136:ASP:C	2.54	0.45
1:A:263:ASP:HB3	1:A:271:LYS:NZ	2.32	0.45
1:A:316:LEU:HD22	1:A:316:LEU:N	2.32	0.45
1:B:131:ASN:ND2	2:B:463:HOH:O	2.50	0.45
1:B:175:ASP:CG	1:B:178:LYS:HD3	2.37	0.45
1:B:80:PHE:CE1	1:B:133:ALA:HB3	2.52	0.44
1:B:206:LYS:HE3	1:B:206:LYS:HB2	1.87	0.43
1:A:28:ASN:HB3	1:A:62:LYS:HD2	2.01	0.43
1:B:123:ILE:HD12	2:B:369:HOH:O	2.19	0.43
1:B:47:CYS:HB3	1:B:58:PHE:CE2	2.54	0.43
1:B:280:THR:HA	1:B:295:GLN:O	2.19	0.43
1:B:39:TRP:CE3	1:B:114:ILE:HG13	2.54	0.43
1:A:178:LYS:HB3	1:A:315:TYR:CD1	2.54	0.43
1:B:225:TYR:HA	1:B:299:GLY:O	2.19	0.42
1:A:129:LYS:O	1:A:132:GLU:HG3	2.20	0.42
1:A:242:LEU:HD12	1:A:251:PHE:O	2.20	0.42
1:B:45:VAL:HG22	1:B:46:THR:N	2.35	0.42
1:A:190:SER:HB3	1:A:193:GLU:O	2.20	0.42
1:B:225:TYR:O	1:B:226:LEU:HD13	2.19	0.42
1:B:184:ILE:O	1:B:326:SER:HA	2.19	0.42
1:A:195:ARG:HA	1:A:215:VAL:O	2.21	0.41
1:A:133:ALA:HA	1:B:339:ALA:HB2	2.01	0.41
1:B:54:GLN:HG2	1:B:58:PHE:HB3	2.03	0.41
1:B:90:SER:HA	1:B:116:LYS:O	2.21	0.41
1:B:140:VAL:HB	1:B:141:PRO:HD3	2.03	0.41
1:B:192:ARG:CG	1:B:192:ARG:HH11	2.33	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	339/341 (99%)	322 (95%)	12 (4%)	5 (2%)	12	3
1	B	339/341 (99%)	324 (96%)	14 (4%)	1 (0%)	44	35
All	All	678/682 (99%)	646 (95%)	26 (4%)	6 (1%)	20	10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	12	VAL
1	A	228	GLN
1	A	250	THR
1	A	247	GLN
1	A	288	GLY
1	A	223	ILE

### 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	281/281 (100%)	271 (96%)	10 (4%)	40	32
1	B	281/281 (100%)	274 (98%)	7 (2%)	53	46
All	All	562/562 (100%)	545 (97%)	17 (3%)	46	39

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	8	ASN
1	A	168	GLN
1	A	183	LEU
1	A	201	LEU
1	A	206	LYS
1	A	247	GLN
1	A	287	ASN
1	A	289	GLN
1	A	309	ASN

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Mol	Chain	Res	Type
1	B	62	LYS
1	B	64	ILE
1	B	191	ASP
1	B	192	ARG
1	B	226	LEU
1	B	228	GLN
1	B	241	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	8	ASN
1	A	28	ASN
1	A	74	GLN
1	A	212	ASN
1	A	228	GLN
1	A	232	GLN
1	A	265	ASN
1	A	295	GLN
1	A	309	ASN
1	A	337	ASN
1	B	8	ASN
1	B	121	GLN
1	B	131	ASN
1	B	265	ASN
1	B	295	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

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

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	A	330/341 (96%)	-0.12	12 (3%) 43 48	8, 19, 46, 73	7 (2%)
1	B	334/341 (97%)	-0.23	9 (2%) 55 61	10, 20, 39, 64	14 (4%)
All	All	664/682 (97%)	-0.17	21 (3%) 48 53	8, 19, 43, 73	21 (3%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	TYR	6.3
1	B	53	GLY	4.8
1	A	284	SER	4.4
1	A	292	PRO	4.3
1	A	290	PRO	4.1
1	B	52	PRO	4.1
1	A	291	TYR	4.1
1	A	251	PHE	3.7
1	B	258	THR	3.4
1	A	135	GLY	3.2
1	B	51	ARG	3.1
1	B	286	ALA	3.0
1	A	241	GLU	2.9
1	B	251	PHE	2.7
1	B	242	LEU	2.5
1	A	289	GLN	2.4
1	A	232	GLN	2.3
1	B	288	GLY	2.3
1	A	239	GLN	2.2
1	A	205	GLY	2.2
1	B	259	SER	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.