



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:06 AM EDT

PDB ID : 2F68 / pdb_00002f68
Title : Crystal structure of collagen adhesin (CNA) from S. aureus
Authors : Zong, Y.; Narayana, S.V.L.
Deposited on : 2005-11-28
Resolution : 1.95 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

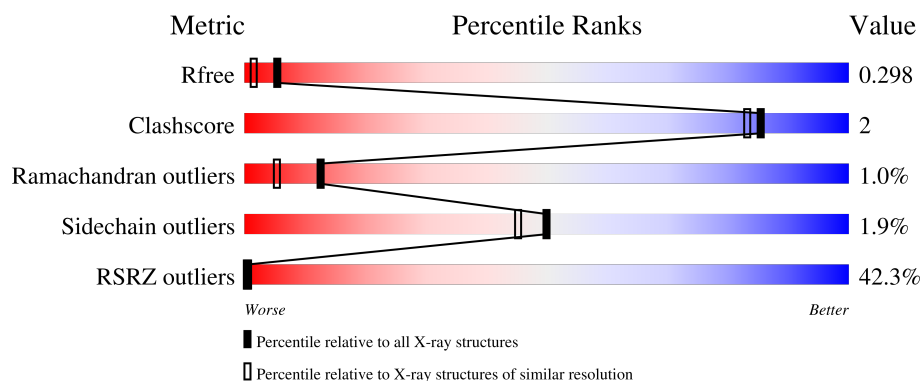
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 of 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 $\leq 5\%$. 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	X	313	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2482 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 Collagen adhesin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	300	Total	C	N	O	S	0	0	0
			2316	1437	394	482	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	22	HIS	-	expression tag	UNP Q53654
X	23	HIS	-	expression tag	UNP Q53654
X	24	HIS	-	expression tag	UNP Q53654
X	25	HIS	-	expression tag	UNP Q53654
X	26	HIS	-	expression tag	UNP Q53654
X	27	HIS	-	expression tag	UNP Q53654
X	28	GLY	-	cloning artifact	UNP Q53654
X	29	SER	-	cloning artifact	UNP Q53654

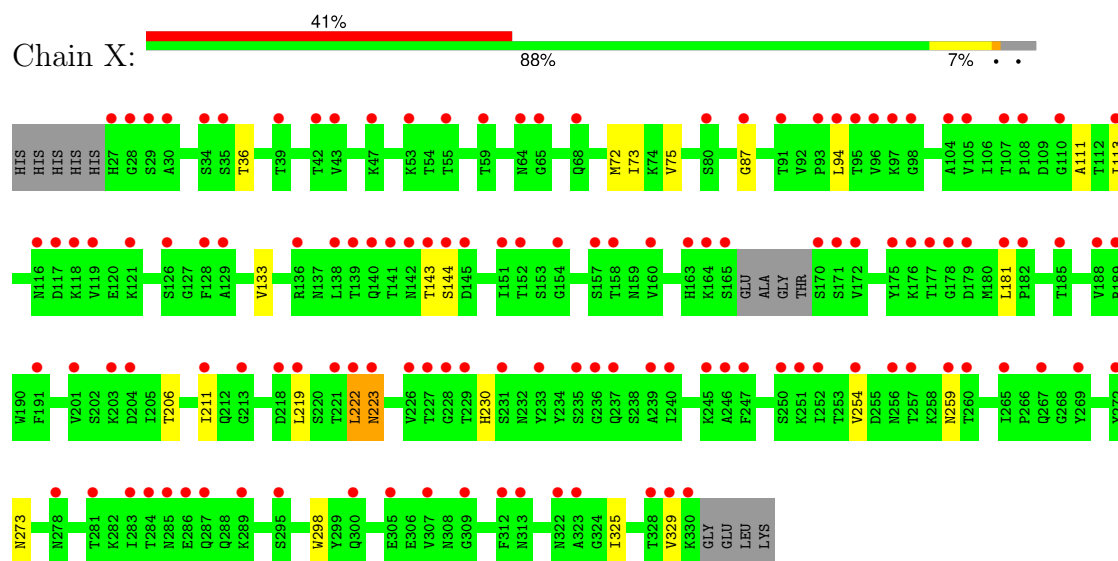
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	166	Total	O	0	0
			166	166		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Collagen adhesin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.98Å 106.43Å 44.08Å 90.00° 116.44° 90.00°	Depositor
Resolution (Å)	52.00 – 1.95 52.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.0 (52.00-1.95) 96.2 (52.00-1.95)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.93 (at 1.86Å)	Xtriage
Refinement program	CNS, REFMAC 5.1.24	Depositor
R, R_{free}	0.195 , 0.253 0.300 , 0.298	Depositor DCC
R_{free} test set	1422 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	2482	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	X	0.44	0/2355	0.65	0/3190

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 [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	X	2316	0	2246	10	0
2	X	166	0	0	1	0
All	All	2482	0	2246	10	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 2.

All (10) 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:X:230:HIS:HD2	1:X:273:ASN:HD21	1.54	0.56
1:X:211:ILE:HB	1:X:259:ASN:HB3	1.92	0.51
1:X:36:THR:HG23	2:X:412:HOH:O	2.13	0.48
1:X:75:VAL:HB	1:X:111:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:87:GLY:HA2	1:X:133:VAL:HG12	1.96	0.48
1:X:219:LEU:HD13	1:X:254:VAL:HG11	1.95	0.48
1:X:206:THR:HB	1:X:298:TRP:HB2	1.98	0.45
1:X:72:MET:HA	1:X:113:ILE:O	2.17	0.45
1:X:94:LEU:HD12	1:X:325:ILE:HB	2.01	0.42
1:X:73:ILE:HB	1:X:113:ILE:HB	2.03	0.41

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	X	296/313 (95%)	285 (96%)	8 (3%)	3 (1%)	12 5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	223	ASN
1	X	144	SER
1	X	222	LEU

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	X	264/274 (96%)	259 (98%)	5 (2%)	50 45

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	143	THR
1	X	181	LEU
1	X	222	LEU
1	X	223	ASN
1	X	329	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	69	ASN
1	X	155	ASN
1	X	223	ASN
1	X	225	ASN
1	X	230	HIS
1	X	267	GLN
1	X	313	ASN
1	X	314	HIS

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 oligosaccharides 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, 95th 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	X	300/313 (95%)	1.96	127 (42%) 0 0	18, 26, 44, 51	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	143	THR	6.7
1	X	185	THR	5.9
1	X	222	LEU	5.5
1	X	330	LYS	4.9
1	X	141	THR	4.6
1	X	221	THR	4.5
1	X	329	VAL	4.4
1	X	245	LYS	4.4
1	X	144	SER	4.2
1	X	142	ASN	4.2
1	X	171	SER	4.1
1	X	64	ASN	4.1
1	X	236	GLY	4.0
1	X	95	THR	3.9
1	X	164	LYS	3.9
1	X	181	LEU	3.9
1	X	251	LYS	3.8
1	X	165	SER	3.7
1	X	250	SER	3.7
1	X	43	VAL	3.7
1	X	140	GLN	3.6
1	X	229	THR	3.6
1	X	170	SER	3.6
1	X	231	SER	3.6
1	X	235	SER	3.6
1	X	239	ALA	3.5
1	X	309	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	X	34	SER	3.5
1	X	27	HIS	3.5
1	X	228	GLY	3.4
1	X	284	THR	3.4
1	X	28	GLY	3.4
1	X	154	GLY	3.4
1	X	163	HIS	3.3
1	X	151	ILE	3.3
1	X	204	ASP	3.3
1	X	118	LYS	3.2
1	X	30	ALA	3.2
1	X	129	ALA	3.2
1	X	35	SER	3.2
1	X	157	SER	3.1
1	X	94	LEU	3.0
1	X	39	THR	3.0
1	X	145	ASP	3.0
1	X	213	GLY	3.0
1	X	138	LEU	2.9
1	X	42	THR	2.9
1	X	87	GLY	2.9
1	X	98	GLY	2.9
1	X	201	VAL	2.9
1	X	116	ASN	2.9
1	X	223	ASN	2.9
1	X	252	ILE	2.9
1	X	172	VAL	2.8
1	X	278	ASN	2.8
1	X	322	ASN	2.8
1	X	53	LYS	2.8
1	X	175	TYR	2.8
1	X	139	THR	2.8
1	X	96	VAL	2.8
1	X	227	THR	2.8
1	X	29	SER	2.7
1	X	176	LYS	2.7
1	X	281	THR	2.7
1	X	233	TYR	2.6
1	X	158	THR	2.6
1	X	97	LYS	2.6
1	X	295	SER	2.6
1	X	182	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	X	80	SER	2.6
1	X	117	ASP	2.6
1	X	219	LEU	2.6
1	X	283	ILE	2.6
1	X	107	THR	2.6
1	X	65	GLY	2.5
1	X	240	ILE	2.5
1	X	328	THR	2.5
1	X	218	ASP	2.5
1	X	285	ASN	2.5
1	X	105	VAL	2.5
1	X	91	THR	2.5
1	X	226	VAL	2.4
1	X	256	ASN	2.4
1	X	237	GLN	2.4
1	X	121	LYS	2.4
1	X	113	ILE	2.4
1	X	104	ALA	2.4
1	X	178	GLY	2.4
1	X	272	TYR	2.4
1	X	108	PRO	2.4
1	X	110	GLY	2.4
1	X	119	VAL	2.4
1	X	203	LYS	2.4
1	X	300	GLN	2.3
1	X	246	ALA	2.3
1	X	305	GLU	2.3
1	X	59	THR	2.3
1	X	247	PHE	2.3
1	X	126	SER	2.3
1	X	160	VAL	2.3
1	X	307	VAL	2.3
1	X	152	THR	2.3
1	X	47	LYS	2.3
1	X	136	ARG	2.2
1	X	189	ARG	2.2
1	X	323	ALA	2.2
1	X	179	ASP	2.2
1	X	211	ILE	2.2
1	X	265	ILE	2.2
1	X	177	THR	2.2
1	X	260	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	68	GLN	2.2
1	X	287	GLN	2.2
1	X	259	ASN	2.2
1	X	313	ASN	2.2
1	X	257	THR	2.2
1	X	254	VAL	2.2
1	X	267	GLN	2.2
1	X	269	TYR	2.1
1	X	55	THR	2.1
1	X	188	VAL	2.1
1	X	289	LYS	2.1
1	X	286	GLU	2.1
1	X	128	PHE	2.1
1	X	312	PHE	2.1
1	X	93	PRO	2.1
1	X	191	PHE	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 oligosaccharides 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.