



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:49 pm BST

PDB ID : 1D2P
Title : CRYSTAL STRUCTURE OF TWO B REPEAT UNITS (B1B2) OF THE
COLLAGEN BINDING PROTEIN (CNA) OF STAPHYLOCOCCUS AU-
REUS
Authors : Deivanayagam, C.C.S.; Rich, R.L.; Hook, M.; Narayana, S.V.L.
Deposited on : 1999-09-25
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
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

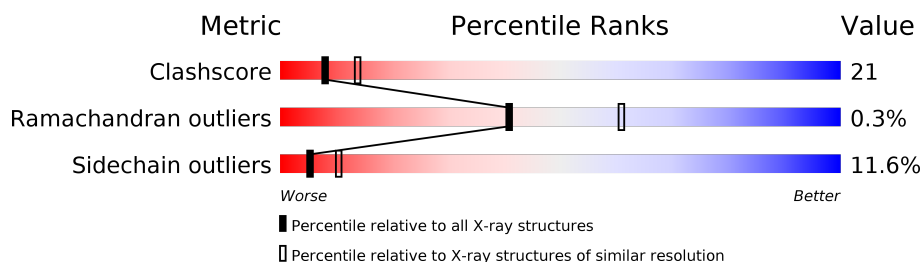
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 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	373	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3061 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	A	373	Total	C	N	O	S	0	0	0
			2986	1847	499	638	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	539	SER	ILE	CONFLICT	UNP Q53654
A	540	ILE	SER	CONFLICT	UNP Q53654
A	715	THR	VAL	CONFLICT	UNP Q53654
A	726	SER	ILE	CONFLICT	UNP Q53654
A	727	ILE	SER	CONFLICT	UNP Q53654
A	753	ASN	ASP	CONFLICT	UNP Q53654
A	902	THR	VAL	CONFLICT	UNP Q53654

- Molecule 2 is water.

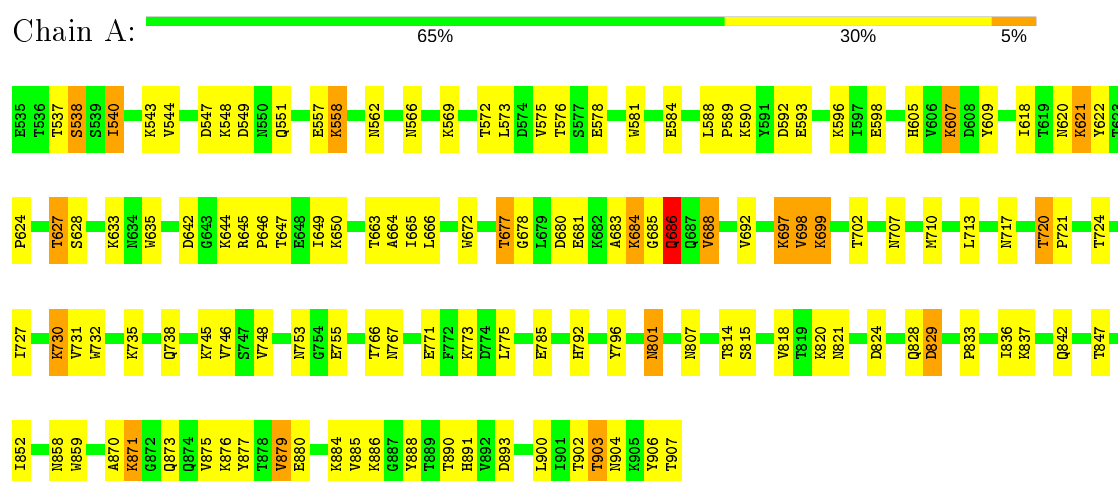
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	75	Total	O	0	0
			75	75		

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: COLLAGEN ADHESIN



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, α , β , γ	42.39 Å 79.42 Å 130.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.50	Depositor
% Data completeness (in resolution range)	97.2 (19.95-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.185 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3061	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

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	A	0.37	0/3040	0.63	0/4125

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	A	2986	0	2870	125	0
2	A	75	0	0	5	0
All	All	3061	0	2870	125	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 21.

All (125) 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:730:LYS:NZ	1:A:807:ASN:HD22	1.45	1.12
1:A:727:ILE:HG22	1:A:771:GLU:HG3	1.37	1.02
1:A:699:LYS:HE3	1:A:699:LYS:HA	1.42	1.00
1:A:730:LYS:CE	1:A:807:ASN:HD22	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:LYS:NZ	1:A:807:ASN:ND2	2.27	0.83
1:A:792:HIS:NE2	1:A:814:THR:HG21	1.92	0.83
1:A:730:LYS:HE3	1:A:807:ASN:ND2	1.93	0.83
1:A:730:LYS:CE	1:A:807:ASN:ND2	2.44	0.81
1:A:842:GLN:HG2	1:A:847:THR:HG22	1.64	0.78
1:A:730:LYS:HZ2	1:A:807:ASN:HD22	1.31	0.77
1:A:605:HIS:CE1	1:A:627:THR:HG21	2.18	0.77
1:A:609:TYR:O	1:A:627:THR:HG22	1.86	0.76
1:A:884:LYS:HB2	1:A:884:LYS:NZ	2.00	0.75
1:A:537:THR:HG22	1:A:538:SER:H	1.52	0.74
1:A:820:LYS:NZ	1:A:904:ASN:HB2	2.03	0.73
1:A:543:LYS:NZ	1:A:620:ASN:OD1	2.20	0.73
1:A:683:ALA:O	1:A:684:LYS:HG2	1.89	0.72
1:A:796:TYR:O	1:A:814:THR:HG22	1.90	0.71
1:A:633:LYS:HE3	1:A:717:ASN:OD1	1.91	0.70
1:A:753:ASN:ND2	1:A:785:GLU:H	1.89	0.69
1:A:633:LYS:NZ	1:A:717:ASN:OD1	2.27	0.67
1:A:753:ASN:HD21	1:A:785:GLU:H	1.42	0.67
1:A:884:LYS:HB2	1:A:884:LYS:HZ2	1.60	0.67
1:A:663:THR:CG2	1:A:664:ALA:N	2.59	0.65
1:A:537:THR:HG22	1:A:538:SER:N	2.13	0.64
1:A:885:VAL:HG23	1:A:888:TYR:HB2	1.78	0.64
1:A:633:LYS:CE	1:A:717:ASN:OD1	2.46	0.64
1:A:727:ILE:CG2	1:A:771:GLU:HG3	2.24	0.64
1:A:566:ASN:ND2	1:A:598:GLU:H	1.95	0.63
1:A:692:VAL:CG2	1:A:713:LEU:HD13	2.28	0.63
1:A:566:ASN:HD21	1:A:598:GLU:H	1.45	0.63
1:A:650:LYS:HG2	1:A:665:ILE:HG13	1.81	0.62
1:A:820:LYS:HE3	1:A:836:ILE:HD13	1.81	0.62
1:A:833:PRO:HG3	1:A:885:VAL:HG11	1.82	0.62
1:A:543:LYS:CE	1:A:620:ASN:OD1	2.51	0.59
1:A:633:LYS:HB3	1:A:672:TRP:HB3	1.86	0.58
1:A:663:THR:HG22	1:A:664:ALA:N	2.19	0.58
1:A:543:LYS:HE3	1:A:620:ASN:OD1	2.04	0.57
1:A:842:GLN:HB3	1:A:877:TYR:CE1	2.39	0.57
1:A:685:GLY:O	1:A:686:GLN:HB3	2.05	0.57
1:A:820:LYS:HZ3	1:A:904:ASN:HB2	1.68	0.57
1:A:686:GLN:O	1:A:686:GLN:HG2	2.05	0.57
1:A:730:LYS:HZ1	1:A:807:ASN:HD22	1.46	0.56
1:A:886:LYS:N	1:A:886:LYS:HD2	2.20	0.56
1:A:820:LYS:HD2	1:A:902:THR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:LYS:HB2	1:A:576:THR:HG22	1.87	0.55
1:A:820:LYS:NZ	1:A:904:ASN:OD1	2.41	0.54
1:A:879:VAL:HG22	1:A:900:LEU:HD13	1.87	0.54
1:A:635:TRP:CD2	1:A:645:ARG:HD2	2.43	0.54
1:A:649:ILE:HD11	1:A:666:LEU:HD12	1.90	0.54
1:A:677:THR:CG2	1:A:678:GLY:N	2.71	0.54
1:A:605:HIS:HE1	1:A:627:THR:HG21	1.72	0.53
1:A:710:MET:HE2	2:A:997:HOH:O	2.08	0.53
1:A:820:LYS:HZ1	1:A:904:ASN:HB2	1.75	0.52
1:A:890:THR:OG1	1:A:904:ASN:ND2	2.44	0.51
1:A:684:LYS:CG	1:A:684:LYS:O	2.59	0.51
1:A:665:ILE:HD12	1:A:665:ILE:N	2.26	0.50
1:A:681:GLU:O	1:A:688:VAL:HG13	2.12	0.50
1:A:820:LYS:NZ	1:A:904:ASN:CB	2.75	0.50
1:A:621:LYS:O	1:A:621:LYS:HG3	2.12	0.49
1:A:730:LYS:HD3	1:A:732:TRP:CZ2	2.48	0.49
1:A:572:THR:HG22	1:A:573:LEU:N	2.26	0.49
1:A:576:THR:OG1	1:A:578:GLU:HB2	2.13	0.48
1:A:677:THR:HG23	1:A:678:GLY:N	2.28	0.48
1:A:735:LYS:HB2	1:A:738:GLN:HB2	1.95	0.48
1:A:692:VAL:HG23	1:A:713:LEU:HD13	1.95	0.48
1:A:792:HIS:HE1	2:A:981:HOH:O	1.96	0.48
1:A:605:HIS:ND1	1:A:627:THR:HG21	2.28	0.48
1:A:820:LYS:CE	1:A:904:ASN:OD1	2.61	0.48
1:A:684:LYS:NZ	1:A:684:LYS:HB3	2.28	0.47
1:A:730:LYS:HZ1	1:A:807:ASN:ND2	2.04	0.47
1:A:890:THR:HG23	1:A:904:ASN:HD21	1.79	0.47
1:A:821:ASN:HB3	1:A:903:THR:HB	1.97	0.47
1:A:547:ASP:HB3	1:A:622:TYR:HB2	1.97	0.47
1:A:730:LYS:HE2	1:A:730:LYS:HB2	1.68	0.47
1:A:540:ILE:HB	1:A:584:GLU:CG	2.46	0.46
1:A:663:THR:CG2	1:A:664:ALA:H	2.29	0.46
1:A:684:LYS:HG3	1:A:684:LYS:O	2.15	0.46
1:A:890:THR:HG23	1:A:904:ASN:ND2	2.29	0.46
1:A:842:GLN:HG2	1:A:847:THR:CG2	2.42	0.46
1:A:558:LYS:CB	1:A:576:THR:HG22	2.45	0.46
1:A:870:ALA:O	1:A:871:LYS:HB2	2.16	0.45
1:A:548:LYS:O	1:A:551:GLN:HG3	2.16	0.45
1:A:642:ASP:O	1:A:644:LYS:HD3	2.16	0.45
1:A:540:ILE:HB	1:A:584:GLU:HG2	1.97	0.45
1:A:785:GLU:OE1	1:A:858:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:ASN:HB2	2:A:988:HOH:O	2.17	0.44
1:A:627:THR:HB	1:A:628:SER:H	1.56	0.44
1:A:663:THR:HG23	1:A:664:ALA:H	1.82	0.44
1:A:814:THR:HB	1:A:815:SER:H	1.69	0.44
1:A:720:THR:HA	1:A:721:PRO:HD3	1.80	0.44
1:A:766:THR:O	1:A:767:ASN:HB2	2.18	0.44
1:A:593:GLU:O	1:A:593:GLU:HG2	2.18	0.44
1:A:590:LYS:CG	1:A:596:LYS:HE3	2.48	0.43
1:A:828:GLN:HG3	1:A:829:ASP:N	2.32	0.43
1:A:730:LYS:HD2	1:A:746:VAL:HG21	1.99	0.43
1:A:871:LYS:N	1:A:871:LYS:HD3	2.34	0.43
1:A:875:VAL:HG12	1:A:876:LYS:N	2.32	0.43
1:A:537:THR:N	1:A:588:LEU:O	2.50	0.43
1:A:618:ILE:HD11	2:A:992:HOH:O	2.19	0.43
1:A:821:ASN:HD22	1:A:903:THR:HB	1.84	0.43
1:A:588:LEU:HA	1:A:589:PRO:HD3	1.91	0.42
1:A:820:LYS:HZ1	1:A:904:ASN:CB	2.33	0.42
1:A:710:MET:CE	2:A:997:HOH:O	2.65	0.42
1:A:837:LYS:HG3	1:A:852:ILE:HD13	2.02	0.42
1:A:605:HIS:NE2	1:A:607:LYS:HD3	2.34	0.42
1:A:824:ASP:HB3	1:A:906:TYR:HB2	2.01	0.42
1:A:537:THR:CG2	1:A:538:SER:H	2.29	0.41
1:A:558:LYS:HB2	1:A:575:VAL:O	2.20	0.41
1:A:646:PRO:HG3	1:A:698:VAL:HG13	2.02	0.41
1:A:890:THR:HA	1:A:904:ASN:HD22	1.85	0.41
1:A:562:ASN:OD1	1:A:569:LYS:HE3	2.20	0.41
1:A:683:ALA:O	1:A:686:GLN:NE2	2.53	0.41
1:A:697:LYS:HB2	1:A:697:LYS:HE2	1.85	0.41
1:A:543:LYS:HB3	1:A:581:TRP:HB3	2.03	0.41
1:A:633:LYS:HZ2	1:A:717:ASN:CG	2.22	0.41
1:A:820:LYS:HB3	1:A:859:TRP:HB3	2.02	0.41
1:A:885:VAL:O	1:A:885:VAL:HG23	2.19	0.41
1:A:622:TYR:CZ	1:A:624:PRO:HG3	2.55	0.41
1:A:707:ASN:HA	1:A:713:LEU:CD2	2.50	0.41
1:A:572:THR:CG2	1:A:573:LEU:N	2.83	0.41
1:A:893:ASP:C	1:A:893:ASP:OD1	2.59	0.41
1:A:543:LYS:HA	1:A:543:LYS:HD2	1.79	0.41
1:A:890:THR:CG2	1:A:904:ASN:HD21	2.33	0.40
1:A:820:LYS:NZ	1:A:904:ASN:CG	2.75	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	371/373 (100%)	353 (95%)	17 (5%)	1 (0%)	41 61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	686	GLN

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	337/337 (100%)	298 (88%)	39 (12%)	5 10

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	538	SER
1	A	540	ILE
1	A	544	VAL
1	A	549	ASP
1	A	557	GLU
1	A	558	LYS
1	A	592	ASP
1	A	607	LYS
1	A	621	LYS
1	A	627	THR

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Mol	Chain	Res	Type
1	A	647	THR
1	A	677	THR
1	A	680	ASP
1	A	684	LYS
1	A	686	GLN
1	A	688	VAL
1	A	697	LYS
1	A	698	VAL
1	A	699	LYS
1	A	702	THR
1	A	720	THR
1	A	724	THR
1	A	730	LYS
1	A	731	VAL
1	A	745	LYS
1	A	748	VAL
1	A	755	GLU
1	A	773	LYS
1	A	775	LEU
1	A	801	ASN
1	A	818	VAL
1	A	829	ASP
1	A	871	LYS
1	A	873	GLN
1	A	879	VAL
1	A	880	GLU
1	A	891	HIS
1	A	903	THR
1	A	907	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	551	GLN
1	A	566	ASN
1	A	580	ASN
1	A	639	ASN
1	A	674	HIS
1	A	686	GLN
1	A	738	GLN
1	A	753	ASN
1	A	801	ASN

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Mol	Chain	Res	Type
1	A	807	ASN
1	A	821	ASN
1	A	828	GLN
1	A	842	GLN
1	A	861	HIS
1	A	873	GLN
1	A	874	GLN
1	A	891	HIS
1	A	895	ASN

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](#)

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 [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.