



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2VR3 / pdb_00002vr3
Title : Structural and Biochemical Characterization of Fibrinogen binding to ClfA from *Staphylococcus aureus*
Authors : Ganesh, V.K.; Rivera, J.J.; Smeds, E.; Bowden, M.G.; Wann, E.R.; Gurudappa, S.; Fitzgerald, J.R.; Hook, M.
Deposited on : 2008-03-25
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

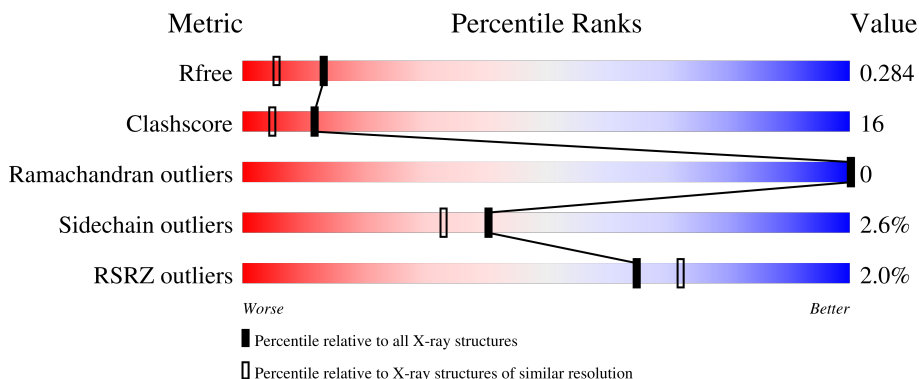
1 Overall quality at a glance

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	A	329	 2% (red), 69% (green), 22% (yellow), 6% (grey)
1	B	329	 2% (red), 68% (green), 25% (yellow), 5% (grey)
2	C	13	 8% (red), 77% (green), 15% (yellow), 8% (grey)
2	D	13	 77% (green), 23% (yellow)

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5226 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 CLUMPING FACTOR A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	308	Total	C	N	O	S	0	0	0
			2269	1432	369	463	5			
1	B	311	Total	C	N	O	S	0	0	1
			2289	1443	371	470	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	CYS	ASP	engineered mutation	UNP Q2G015
A	541	CYS	LYS	engineered mutation	UNP Q2G015
B	327	CYS	ASP	engineered mutation	UNP Q2G015
B	541	CYS	LYS	engineered mutation	UNP Q2G015

- Molecule 2 is a protein called FIBRINOGEN GAMMA-CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	12	Total	C	N	O	0	0	0
			70	42	14	14			
2	D	13	Total	C	N	O	0	0	0
			71	42	14	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	410	ALA	ASP	engineered mutation	UNP P02679
D	410	ALA	ASP	engineered mutation	UNP P02679

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	249	Total	O	0	0
			249	249		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	262	Total 262	O 262	0	0
3	C	10	Total 10	O 10	0	0
3	D	6	Total 6	O 6	0	0

Q899	Q407	A408	G409	A410	V411
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	35.43Å 61.84Å 81.78Å 85.44° 81.84° 82.45°	Depositor
Resolution (Å)	15.00 – 1.95 15.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.2 (15.00-1.95) 92.9 (15.00-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.279 0.213 , 0.284	Depositor DCC
R_{free} test set	941 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtrriage
Anisotropy	0.196	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 87.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5226	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.96% 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	A	0.93	2/2313 (0.1%)	1.15	9/3173 (0.3%)
1	B	0.93	1/2333 (0.0%)	1.15	9/3197 (0.3%)
2	C	1.15	0/69	1.21	1/89 (1.1%)
2	D	1.06	0/70	0.99	0/91
All	All	0.94	3/4785 (0.1%)	1.15	19/6550 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	TYR	CA-C	-6.02	1.46	1.52
1	A	279	VAL	CA-CB	5.93	1.58	1.54
1	B	367	VAL	CA-CB	5.04	1.59	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ASP	CA-C-N	12.27	132.00	119.24
1	A	340	ASP	C-N-CA	12.27	132.00	119.24
1	B	420	THR	N-CA-C	-8.43	97.98	110.46
1	B	409	ALA	CA-C-N	7.45	129.39	120.23
1	B	409	ALA	C-N-CA	7.45	129.39	120.23

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	2269	0	2111	62	0
1	B	2289	0	2125	84	0
2	C	70	0	67	2	0
2	D	71	0	59	3	0
3	A	249	0	0	14	0
3	B	262	0	0	20	0
3	C	10	0	0	0	0
3	D	6	0	0	0	0
All	All	5226	0	4362	143	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 16.

The worst 5 of 143 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:B:386:GLN:HG2	3:B:2157:HOH:O	1.54	1.05
1:B:384:ILE:H	2:D:407:GLN:HE22	1.11	0.97
1:A:279:VAL:H	1:A:314:ASN:HD22	1.11	0.96
1:A:290:SER:O	3:A:2050:HOH:O	1.83	0.95
1:B:281:LYS:NZ	3:B:2045:HOH:O	2.01	0.94

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	300/329 (91%)	289 (96%)	11 (4%)	0	100	100
1	B	305/329 (93%)	291 (95%)	14 (5%)	0	100	100
2	C	10/13 (77%)	10 (100%)	0	0	100	100
2	D	11/13 (85%)	11 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	626/684 (92%)	601 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	242/288 (84%)	234 (97%)	8 (3%)	33	24
1	B	242/288 (84%)	237 (98%)	5 (2%)	47	41
2	C	4/7 (57%)	4 (100%)	0	100	100
2	D	3/7 (43%)	3 (100%)	0	100	100
All	All	491/590 (83%)	478 (97%)	13 (3%)	40	33

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	503	LEU
1	B	304	LEU
1	B	535	SER
1	B	495	ILE
1	B	517	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	515	ASN
1	B	470	ASN
1	A	525	ASN
1	B	468	ASN
1	A	492	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 oligosaccharides 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 [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, 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	A	308/329 (93%)	0.39	7 (2%) 61 68	17, 30, 41, 53	0
1	B	311/329 (94%)	0.33	5 (1%) 70 77	17, 30, 43, 48	0
2	C	12/13 (92%)	0.40	1 (8%) 17 20	18, 25, 44, 49	0
2	D	13/13 (100%)	0.40	0 100 100	18, 23, 44, 49	0
All	All	644/684 (94%)	0.36	13 (2%) 65 72	17, 30, 43, 53	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	539	ILE	2.9
1	A	230	THR	2.7
1	B	303	VAL	2.6
1	A	452	PRO	2.6
2	C	401	HIS	2.5

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.