



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2017 – 06:01 AM EDT

PDB ID : 2DOI  
Title : The X-ray crystallographic structure of the angiogenesis inhibitor, angiostatin, bound to a peptide from the group A streptococcus protein PAM  
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Deposited on : unknown  
Resolution : 3.10 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](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

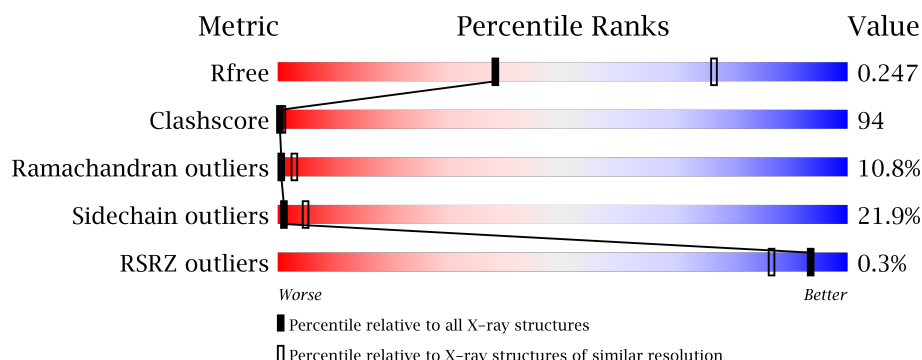
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	234	
1	X	234	
2	B	30	
2	C	30	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3064 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 Angiostatin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	168	Total	C	N	O	S	0	0	0
			1347	824	242	264	17			
1	A	164	Total	C	N	O	S	0	0	0
			1313	803	235	259	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	289	GLU	ASN	ENGINEERED	UNP P00747
A	289	GLU	ASN	ENGINEERED	UNP P00747

- Molecule 2 is a protein called Plasminogen-binding group A streptococcal M-like protein PAM.

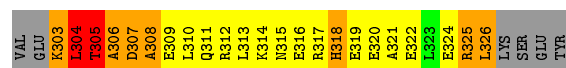
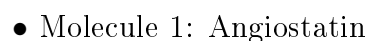
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	24	Total	C	N	O	0	0	0
			202	122	39	41			
2	B	24	Total	C	N	O	0	0	0
			202	122	39	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	330	TYR	-	CLONING ARTIFACT	UNP P49054
B	330	TYR	-	CLONING ARTIFACT	UNP P49054



- Molecule 1: Angiostatin



● Molecule 2: Plasminogen-binding group A streptococcal M-like protein PAM

Chain B:  10% 43% 27% 20%

VAL	GLU	LYS	L304	T305	A306	D307	A308	E309	L310	Q311	R312	L313	K314	R317	H318	E319	E320	A321	E322	L323	E324	R325	L326	K327	SER	GLU	TYR
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.47Å 58.47Å 389.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10 19.96 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-3.10) 85.9 (19.96-2.81)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.202 , 0.296 0.203 , 0.247	Depositor DCC
$R_{free}$ test set	1353 reflections (11.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 14.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.479 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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	1.01	0/1353	1.16	5/1837 (0.3%)
1	X	1.12	2/1387 (0.1%)	1.21	5/1878 (0.3%)
2	B	1.12	0/202	1.35	1/268 (0.4%)
2	C	1.06	0/202	1.38	2/268 (0.7%)
All	All	1.07	2/3144 (0.1%)	1.21	13/4251 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	133	CYS	CB-SG	-6.01	1.72	1.82
1	X	187	CYS	CB-SG	-5.07	1.73	1.81

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	326	LEU	CA-CB-CG	8.21	134.17	115.30
1	X	128	LEU	CA-CB-CG	-6.39	100.60	115.30
1	X	185	LEU	CB-CG-CD2	-6.25	100.38	111.00
2	C	304	LEU	CB-CG-CD1	6.14	121.45	111.00
1	A	181	THR	CB-CA-C	-6.07	95.22	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	LYS	Peptide

## 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	1313	0	1182	254	0
1	X	1347	0	1225	257	0
2	B	202	0	202	37	0
2	C	202	0	202	37	0
All	All	3064	0	2811	552	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 94.

The worst 5 of 552 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:187:CYS:HB2	1:A:213:ASN:ND2	1.62	1.12
1:X:103:ILE:HD12	1:X:103:ILE:H	1.08	1.11
1:X:195:PRO:O	1:X:196:HIS:HD2	1.32	1.10
1:X:224:PRO:CG	1:X:240:ILE:HD12	1.81	1.10
1:X:133:CYS:O	1:X:134:ARG:HD3	1.51	1.08

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	162/234 (69%)	113 (70%)	36 (22%)	13 (8%)	1	6
1	X	164/234 (70%)	112 (68%)	32 (20%)	20 (12%)	0	2
2	B	22/30 (73%)	14 (64%)	7 (32%)	1 (4%)	3	17
2	C	22/30 (73%)	9 (41%)	7 (32%)	6 (27%)	0	0
All	All	370/528 (70%)	248 (67%)	82 (22%)	40 (11%)	0	3

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	121	ALA
1	X	127	GLY
1	X	159	ILE
1	X	163	GLU
1	X	169	CYS

### 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	148/212 (70%)	117 (79%)	31 (21%)	1	6
1	X	153/212 (72%)	118 (77%)	35 (23%)	1	4
2	B	21/27 (78%)	15 (71%)	6 (29%)	0	1
2	C	21/27 (78%)	18 (86%)	3 (14%)	4	17
All	All	343/478 (72%)	268 (78%)	75 (22%)	1	5

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	297	CYS
1	A	103	ILE
2	B	304	LEU
1	X	298	LYS
1	A	82	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	315	ASN
2	C	318	HIS
1	A	209	ASN
2	C	311	GLN
1	A	138	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 [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	A	164/234 (70%)	-0.86	1 (0%) 89 77	10, 33, 58, 81	0
1	X	168/234 (71%)	-0.91	0 100 100	11, 33, 55, 66	0
2	B	24/30 (80%)	-0.88	0 100 100	15, 43, 52, 70	0
2	C	24/30 (80%)	-0.84	0 100 100	13, 33, 55, 60	0
All	All	380/528 (71%)	-0.88	1 (0%) 93 86	10, 33, 58, 81	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	THR	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.