



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3PR7 / pdb\_00003pr7  
Title : Multi-functional and mechanosensitive receptor binding activity of the  
Moraxella catarrhalis adhesin UspA1  
Authors : Agnew, C.R.J.; Zaccai, N.R.; Connors, R.; Brady, R.L.  
Deposited on : 2010-11-29  
Resolution : 2.94 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

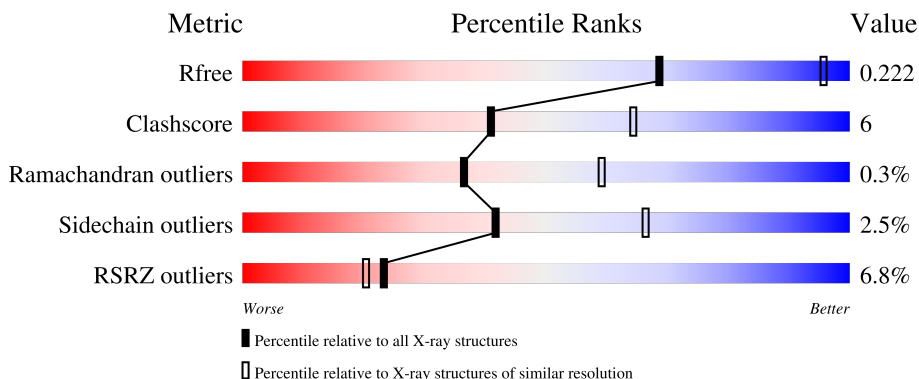
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.94 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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  $\geq 3$ , 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	311	 7% 82% 11% • 6%
1	B	311	 5% 82% 11% • 6%
1	C	311	 8% 80% 13% • 6%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 6177 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 UspA1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	292	2044	1225	377	442	0	1	0
1	B	292	2044	1225	377	442	0	1	0
1	C	292	2044	1225	377	442	0	1	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	LYS	-	expression tag	UNP Q9XD56
A	347	HIS	-	expression tag	UNP Q9XD56
A	348	HIS	-	expression tag	UNP Q9XD56
A	349	HIS	-	expression tag	UNP Q9XD56
A	350	HIS	-	expression tag	UNP Q9XD56
A	351	HIS	-	expression tag	UNP Q9XD56
A	352	HIS	-	expression tag	UNP Q9XD56
B	346	LYS	-	expression tag	UNP Q9XD56
B	347	HIS	-	expression tag	UNP Q9XD56
B	348	HIS	-	expression tag	UNP Q9XD56
B	349	HIS	-	expression tag	UNP Q9XD56
B	350	HIS	-	expression tag	UNP Q9XD56
B	351	HIS	-	expression tag	UNP Q9XD56
B	352	HIS	-	expression tag	UNP Q9XD56
C	346	LYS	-	expression tag	UNP Q9XD56
C	347	HIS	-	expression tag	UNP Q9XD56
C	348	HIS	-	expression tag	UNP Q9XD56
C	349	HIS	-	expression tag	UNP Q9XD56
C	350	HIS	-	expression tag	UNP Q9XD56
C	351	HIS	-	expression tag	UNP Q9XD56
C	352	HIS	-	expression tag	UNP Q9XD56

- Molecule 2 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	A	14	Total 14	O 14	0	0
2	B	7	Total 7	O 7	0	0
2	C	24	Total 24	O 24	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.22Å 118.22Å 176.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.60 – 2.94 29.60 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.60-2.94) 99.8 (29.60-2.94)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.55 (at 2.96Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.203 , 0.216 0.209 , 0.222	Depositor DCC
$R_{free}$ test set	1503 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtrriage
Anisotropy	0.110	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6177	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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 [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	0.43	1/2065 (0.0%)	0.75	2/2786 (0.1%)
1	B	0.40	0/2065	0.75	3/2786 (0.1%)
1	C	0.61	1/2065 (0.0%)	0.82	9/2786 (0.3%)
All	All	0.49	2/6195 (0.0%)	0.78	14/8358 (0.2%)

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	232	GLU	CD-OE2	20.02	1.63	1.25
1	A	338	HIS	CE1-NE2	6.74	1.39	1.32

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	ARG	NE-CZ-NH2	9.31	127.58	119.20
1	C	197	ARG	NE-CZ-NH1	-9.01	112.50	121.50
1	C	232	GLU	CB-CG-CD	7.28	124.97	112.60
1	C	197	ARG	CD-NE-CZ	7.10	134.34	124.40
1	C	232	GLU	CA-CB-CG	-5.60	102.89	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	232	GLU	Sidechain

## 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	2044	0	1963	32	0
1	B	2044	0	1963	29	0
1	C	2044	0	1963	33	0
2	A	14	0	0	0	0
2	B	7	0	0	0	0
2	C	24	0	0	0	0
All	All	6177	0	5889	78	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 6.

The worst 5 of 78 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:72:THR:HG21	1:B:75:GLY:HA3	1.45	0.96
1:B:72:THR:HG21	1:C:75:GLY:HA3	1.47	0.93
1:A:75:GLY:HA3	1:C:72:THR:HG21	1.49	0.93
1:A:158:ILE:HG22	1:A:159:GLU:N	2.10	0.67
1:B:158:ILE:HG22	1:B:159:GLU:N	2.09	0.66

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	291/311 (94%)	278 (96%)	12 (4%)	1 (0%)	36	59
1	B	291/311 (94%)	276 (95%)	14 (5%)	1 (0%)	36	59
1	C	291/311 (94%)	278 (96%)	12 (4%)	1 (0%)	36	59
All	All	873/933 (94%)	832 (95%)	38 (4%)	3 (0%)	36	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	SER
1	B	105	SER
1	C	105	SER

### 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	204/218 (94%)	199 (98%)	5 (2%)	42	66
1	B	204/218 (94%)	197 (97%)	7 (3%)	32	58
1	C	204/218 (94%)	198 (97%)	6 (3%)	37	62
All	All	612/654 (94%)	594 (97%)	18 (3%)	42	62

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	163	VAL
1	C	223[B]	LEU
1	C	223[A]	LEU
1	B	163	VAL
1	C	98	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	240	ASN
1	C	248	GLN
1	B	241	ASN
1	C	261	ASN
1	C	225	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, 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	292/311 (93%)	0.33	21 (7%) 21 19	25, 58, 112, 159	1 (0%)
1	B	292/311 (93%)	0.31	14 (4%) 35 29	28, 62, 114, 144	1 (0%)
1	C	292/311 (93%)	0.33	25 (8%) 16 14	26, 52, 121, 151	1 (0%)
All	All	876/933 (93%)	0.32	60 (6%) 23 20	25, 58, 115, 159	3 (0%)

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	GLY	8.4
1	C	54	ALA	6.2
1	B	345	ALA	5.2
1	A	54	ALA	5.1
1	B	54	ALA	5.1

### 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.