



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:21 AM UTC

PDB ID : 1AW7 / pdb_00001aw7
Title : Q136A MUTANT OF TOXIC SHOCK SYNDROME TOXIN-1 FROM S. AU-REUS
Authors : Earhart, C.A.; Mitchell, D.T.; Murray, D.L.; Pinheiro, D.M.; Matsumura, M.; Schlievert, P.M.; Ohlendorf, D.H.
Deposited on : 1997-10-11
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

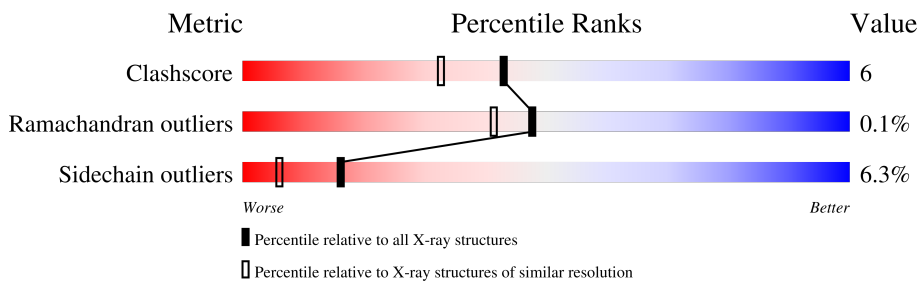
1 Overall quality at a glance

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))
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	194	 75% 21% •
1	B	194	 70% 25% 5% •
1	C	194	 77% 21% •
1	D	194	 74% 23% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6539 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 TOXIC SHOCK SYNDROME TOXIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	1	0
			1562	994	256	310	2			
1	B	194	Total	C	N	O	S	0	1	0
			1562	994	256	310	2			
1	C	194	Total	C	N	O	S	0	1	0
			1562	994	256	310	2			
1	D	194	Total	C	N	O	S	0	1	0
			1562	994	256	310	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	TRP	GLY	SEE REMARK 999	UNP P06886
A	136	ALA	GLN	engineered mutation	UNP P06886
B	316	TRP	GLY	SEE REMARK 999	UNP P06886
B	336	ALA	GLN	engineered mutation	UNP P06886
C	516	TRP	GLY	SEE REMARK 999	UNP P06886
C	536	ALA	GLN	engineered mutation	UNP P06886
D	716	TRP	GLY	SEE REMARK 999	UNP P06886
D	736	ALA	GLN	engineered mutation	UNP P06886

- Molecule 2 is water.

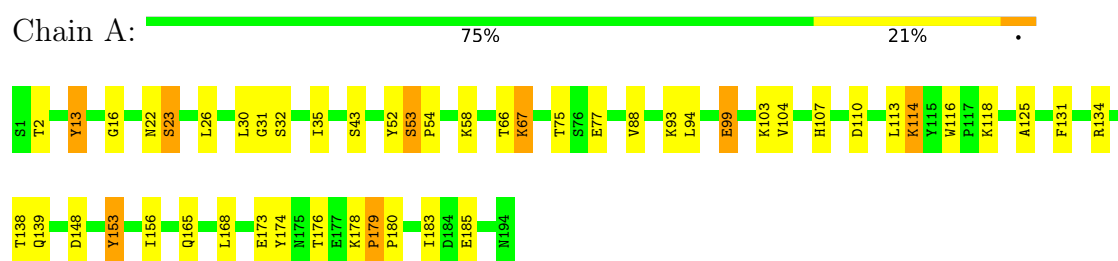
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	79	Total	O	0	0
			79	79		
2	C	64	Total	O	0	0
			64	64		
2	D	70	Total	O	0	0
			70	70		

3 Residue-property plots [i](#)

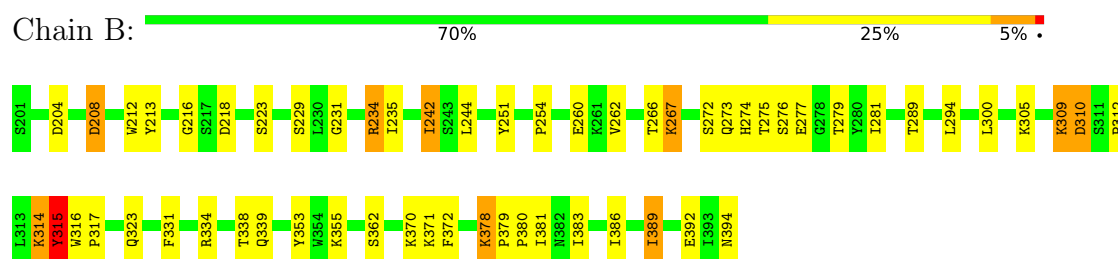
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

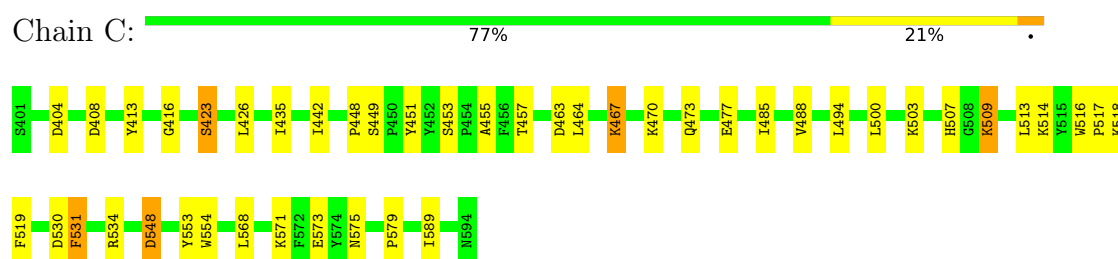
• Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1



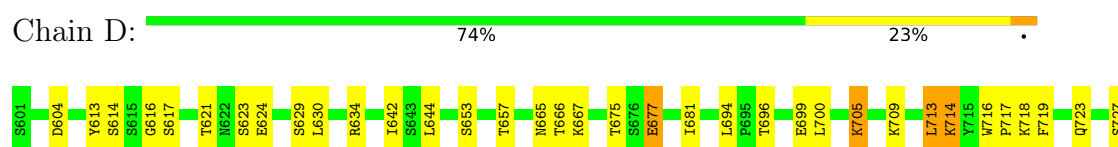
• Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1



• Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1



• Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1



F731	E732	I733	R734
H741	G742	L743	
Y753	W754	K755	
Q765	S766		
K778	P779	P780	
	I789		
		V794	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.63Å 99.28Å 41.33Å 88.50° 93.30° 91.10°	Depositor
Resolution (Å)	20.00 – 1.95	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6539	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

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	1.51	9/1603 (0.6%)	1.41	19/2168 (0.9%)
1	B	1.52	11/1603 (0.7%)	1.40	16/2168 (0.7%)
1	C	1.47	7/1603 (0.4%)	1.39	15/2168 (0.7%)
1	D	1.44	11/1603 (0.7%)	1.38	11/2168 (0.5%)
All	All	1.48	38/6412 (0.6%)	1.39	61/8672 (0.7%)

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	2
1	B	0	2
All	All	0	4

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	642	ILE	CA-CB	8.10	1.64	1.54
1	B	242	ILE	CA-CB	7.69	1.65	1.54
1	C	548	ASP	CA-C	6.91	1.62	1.52
1	D	666	THR	CA-CB	6.84	1.64	1.53
1	A	43	SER	C-O	6.79	1.32	1.24

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	404	ASP	N-CA-C	7.47	120.30	111.71
1	A	31	GLY	N-CA-C	7.44	125.70	114.61
1	A	114	LYS	N-CA-C	7.34	120.48	108.52
1	C	531[A]	PHE	N-CA-C	7.34	120.15	111.71
1	C	531[B]	PHE	N-CA-C	7.34	120.15	111.71

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	TYR	Sidechain
1	A	174	TYR	Sidechain
1	B	251	TYR	Sidechain
1	B	315	TYR	Sidechain

5.2 Too-close contacts

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	1562	0	1545	15	0
1	B	1562	0	1542	23	0
1	C	1562	0	1542	16	0
1	D	1562	0	1542	23	0
2	A	78	0	0	4	0
2	B	79	0	0	0	0
2	C	64	0	0	0	0
2	D	70	0	0	0	0
All	All	6539	0	6171	77	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 77 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:C:416:GLY:O	1:C:467:LYS:HE2	1.72	0.88
1:C:467:LYS:HE3	1:C:531[A]:PHE:CE2	2.21	0.75
1:B:216:GLY:O	1:B:267:LYS:HE2	1.93	0.68
2:A:196:HOH:O	1:B:274:HIS:HE1	1.74	0.68
1:D:616:GLY:O	1:D:667:LYS:HE2	1.94	0.68

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	193/194 (100%)	187 (97%)	6 (3%)	0	100	100
1	B	193/194 (100%)	187 (97%)	5 (3%)	1 (0%)	24	16
1	C	193/194 (100%)	185 (96%)	8 (4%)	0	100	100
1	D	193/194 (100%)	185 (96%)	8 (4%)	0	100	100
All	All	772/776 (100%)	744 (96%)	27 (4%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	312	PRO

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	180/179 (101%)	169 (94%)	11 (6%)	17	7
1	B	180/179 (101%)	166 (92%)	14 (8%)	11	3
1	C	180/179 (101%)	169 (94%)	11 (6%)	17	7
1	D	180/179 (101%)	170 (94%)	10 (6%)	19	8
All	All	720/716 (101%)	674 (94%)	46 (6%)	16	6

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	473	GLN
1	C	573	GLU
1	C	477	GLU
1	C	509	LYS
1	D	677	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	541	HIS
1	D	723	GLN
1	D	775	ASN
1	D	741	HIS
1	D	665	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

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.