Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 10:20 AM EDT

PDB ID	:	1TS4
Title	:	Q139K MUTANT OF TOXIC SHOCK SYNDROME TOXIN-1 FROM S. AUREUS
Authors	:	Earhart, C.A.; Mitchell, D.T.; Murray, D.L.; Pinheiro, D.M.; Matsumura, M.; Schlievert, P.M.; Ohlendorf, D.H.
Deposited on	:	1997-10-10
Resolution	:	3.40 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 (i) symbol.

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

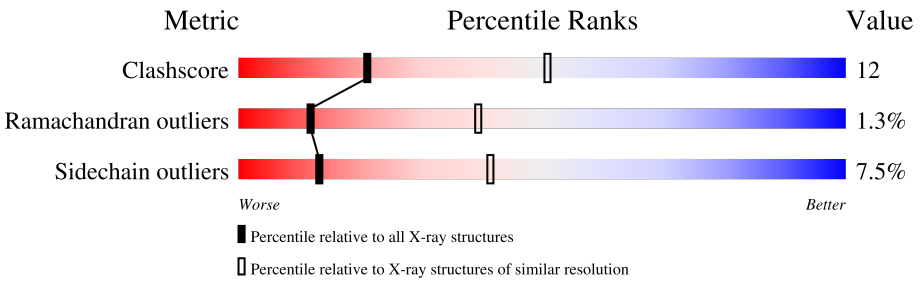
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	194	71% 27% •
1	B	194	72% 24% • •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3118 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
			Total	C	N	O	S			
1	A	194	1559	990	257	310	2	0	0	0
1	B	194	1559	990	257	310	2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	TRP	GLY	SEE REMARK 999	UNP P06886
A	139	LYS	GLN	engineered mutation	UNP P06886
B	316	TRP	GLY	SEE REMARK 999	UNP P06886
B	339	LYS	GLN	engineered mutation	UNP P06886

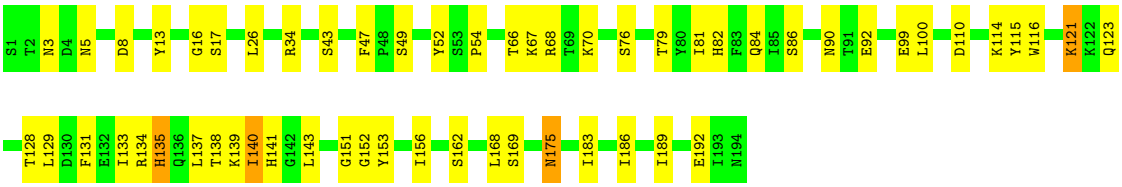
3 Residue-property plots (i)

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.

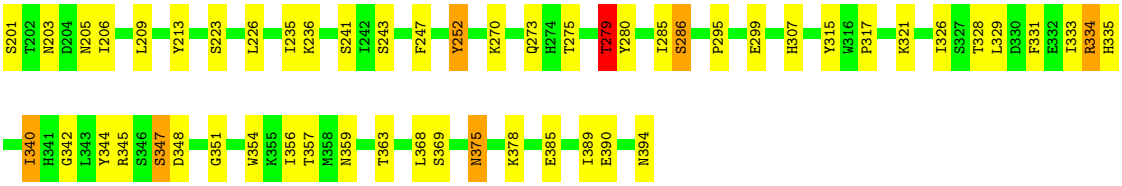
• Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1

Chain A: 71% 27%



• Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1

Chain B: 72% 24%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	152.35Å 152.35Å 142.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.40	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.210 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3118	wwPDB-VP
Average B, all atoms (Å^2)	55.0	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	0.49	0/1595	0.73	0/2156
1	B	0.43	0/1595	0.69	0/2156
All	All	0.46	0/3190	0.71	0/4312

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	1559	0	1548	35	0
1	B	1559	0	1545	40	0
All	All	3118	0	3093	75	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 12.

All (75) 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:100:LEU:HB2	1:A:116:TRP:HZ2	1.32	0.95
1:A:68:ARG:HH21	1:A:82:HIS:CE1	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:CD1	1:A:140:ILE:HG12	2.19	0.78
1:A:100:LEU:HB2	1:A:116:TRP:CZ2	2.20	0.74
1:A:47:PHE:CE1	1:A:86:SER:HA	2.22	0.74
1:A:134:ARG:HA	1:A:137:LEU:HD12	1.71	0.72
1:A:115:TYR:HD1	1:A:140:ILE:HG12	1.53	0.72
1:A:151:GLY:HA2	1:A:168:LEU:O	1.89	0.71
1:A:175:ASN:HD22	1:A:175:ASN:H	1.37	0.71
1:B:275:THR:CG2	1:B:279:THR:HG23	2.22	0.69
1:A:135:HIS:HE1	1:A:139:LYS:HD2	1.58	0.68
1:B:331:PHE:O	1:B:335:HIS:HB2	1.99	0.62
1:B:275:THR:HG21	1:B:279:THR:HG23	1.81	0.61
1:B:375:ASN:HD22	1:B:375:ASN:H	1.48	0.60
1:A:90:ASN:H	1:A:123:GLN:HE21	1.51	0.59
1:B:315:TYR:O	1:B:317:PRO:HD3	2.02	0.58
1:A:3:ASN:OD1	1:A:5:ASN:HB3	2.03	0.57
1:B:247:PHE:CE1	1:B:286:SER:HA	2.40	0.57
1:B:359:ASN:HB2	1:B:385:GLU:O	2.05	0.56
1:A:175:ASN:H	1:A:175:ASN:ND2	2.03	0.56
1:A:47:PHE:HE1	1:A:86:SER:HA	1.65	0.55
1:B:275:THR:HG23	1:B:279:THR:HG23	1.88	0.55
1:B:315:TYR:CE2	1:B:340:ILE:HG12	2.42	0.55
1:B:226:LEU:HD11	1:B:236:LYS:HB2	1.89	0.54
1:A:128:THR:HA	1:A:131:PHE:CE2	2.43	0.54
1:B:328:THR:HA	1:B:331:PHE:CE2	2.44	0.53
1:B:375:ASN:HD22	1:B:375:ASN:N	2.06	0.53
1:B:351:GLY:HA2	1:B:368:LEU:O	2.08	0.53
1:B:201:SER:O	1:B:347:SER:HB3	2.08	0.52
1:B:213:TYR:CG	1:B:334:ARG:HG2	2.44	0.52
1:B:334:ARG:NH1	1:B:368:LEU:HA	2.24	0.52
1:B:357:THR:HA	1:B:363:THR:HG22	1.92	0.52
1:B:201:SER:N	1:B:347:SER:HG	2.09	0.51
1:B:356:ILE:HG12	1:B:389:ILE:HG12	1.93	0.51
1:B:329:LEU:O	1:B:333:ILE:HG13	2.10	0.51
1:A:49:SER:HA	1:A:175:ASN:O	2.10	0.51
1:B:241:SER:HB2	1:B:280:TYR:O	2.11	0.51
1:A:66:THR:OG1	1:A:67:LYS:N	2.46	0.49
1:A:26:LEU:HB2	1:A:34:ARG:O	2.13	0.49
1:A:115:TYR:CE1	1:A:140:ILE:HG12	2.47	0.49
1:B:213:TYR:CD2	1:B:334:ARG:HG2	2.49	0.47
1:A:138:THR:HG22	1:A:143:LEU:O	2.15	0.47
1:A:114:LYS:HB2	1:A:140:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:TYR:CD2	1:B:340:ILE:HG12	2.50	0.47
1:B:340:ILE:HD13	1:B:340:ILE:HA	1.75	0.45
1:B:342:GLY:HA2	1:B:345:ARG:NE	2.32	0.45
1:B:209:LEU:HB3	1:B:344:TYR:CE2	2.52	0.45
1:B:326:ILE:HD12	1:B:378:LYS:O	2.17	0.45
1:A:129:LEU:O	1:A:133:ILE:HG13	2.17	0.44
1:B:331:PHE:CD1	1:B:331:PHE:C	2.91	0.44
1:A:140:ILE:HG22	1:A:141:HIS:CD2	2.53	0.44
1:A:121:LYS:HB3	1:A:121:LYS:NZ	2.33	0.44
1:B:307:HIS:CE1	1:B:394:ASN:HA	2.52	0.44
1:A:140:ILE:HD13	1:A:140:ILE:HA	1.67	0.44
1:A:152:GLY:HA3	1:A:192:GLU:O	2.18	0.43
1:B:279:THR:OG1	1:B:280:TYR:N	2.51	0.43
1:A:17:SER:HB2	1:A:66:THR:O	2.19	0.43
1:A:66:THR:OG1	1:A:84:GLN:HB3	2.19	0.43
1:B:351:GLY:O	1:B:394:ASN:N	2.50	0.42
1:A:183:ILE:HG22	1:A:186:ILE:HD11	2.01	0.42
1:A:13:TYR:CE2	1:A:134:ARG:HD2	2.54	0.42
1:A:47:PHE:CD2	1:A:54:PRO:HG2	2.54	0.42
1:B:203:ASN:ND2	1:B:206:ILE:HG12	2.35	0.42
1:B:354:TRP:HA	1:B:390:GLU:O	2.20	0.42
1:A:156:ILE:HG12	1:A:189:ILE:HG12	2.02	0.42
1:B:307:HIS:NE2	1:B:348:ASP:O	2.53	0.42
1:B:252:TYR:C	1:B:252:TYR:CD1	2.94	0.42
1:B:223:SER:HB3	1:B:235:ILE:CG2	2.50	0.41
1:B:334:ARG:HD2	1:B:368:LEU:HD22	2.01	0.41
1:A:140:ILE:HG22	1:A:141:HIS:CG	2.56	0.41
1:A:183:ILE:HA	1:A:186:ILE:HG13	2.03	0.41
1:B:275:THR:HG22	1:B:279:THR:C	2.41	0.40
1:A:153:TYR:CE1	1:A:192:GLU:HB3	2.56	0.40
1:B:285:ILE:HG23	1:B:285:ILE:O	2.20	0.40
1:B:203:ASN:OD1	1:B:205:ASN:N	2.55	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	192/194 (99%)	174 (91%)	16 (8%)	2 (1%)	15	46
1	B	192/194 (99%)	164 (85%)	25 (13%)	3 (2%)	9	34
All	All	384/388 (99%)	338 (88%)	41 (11%)	5 (1%)	12	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLY
1	A	169	SER
1	B	369	SER
1	B	279	THR
1	B	286	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	180/180 (100%)	165 (92%)	15 (8%)	11	36
1	B	180/180 (100%)	168 (93%)	12 (7%)	16	46
All	All	360/360 (100%)	333 (92%)	27 (8%)	13	41

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	43	SER
1	A	52	TYR
1	A	70	LYS
1	A	76	SER
1	A	79	THR
1	A	81	ILE

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Mol	Chain	Res	Type
1	A	92	GLU
1	A	99	GLU
1	A	110	ASP
1	A	121	LYS
1	A	135	HIS
1	A	140	ILE
1	A	162	SER
1	A	175	ASN
1	B	243	SER
1	B	252	TYR
1	B	270	LYS
1	B	273	GLN
1	B	279	THR
1	B	295	PRO
1	B	299	GLU
1	B	321	LYS
1	B	334	ARG
1	B	340	ILE
1	B	347	SER
1	B	375	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	123	GLN
1	A	135	HIS
1	A	136	GLN
1	A	175	ASN
1	B	336	GLN
1	B	375	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 monosaccharides 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)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.