



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2018 – 08:26 am GMT

PDB ID : 1F77  
Title : STAPHYLOCOCCAL ENTEROTOXIN H DETERMINED TO 2.4 Å RESOLUTION  
Authors : Hakansson, M.; Petersson, K.; Nilsson, H.; Forsberg, G.; Bjork, P.  
Deposited on : 2000-06-26  
Resolution : 2.40 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](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.

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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  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686



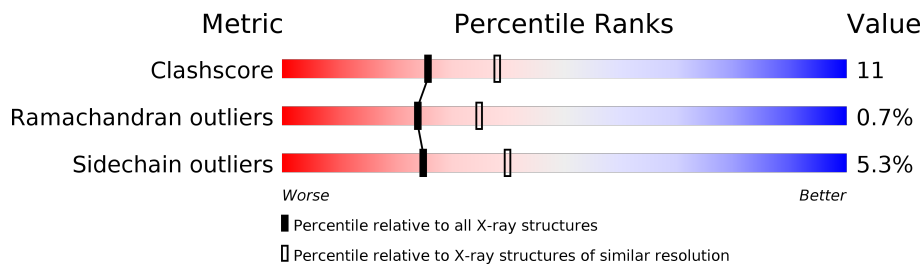
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	122078	3953 (2.40-2.40)
Ramachandran outliers	120005	3894 (2.40-2.40)
Sidechain outliers	119972	3895 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	217	
1	B	217	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	1006	-	-	X	-



## 2 Entry composition [i](#)

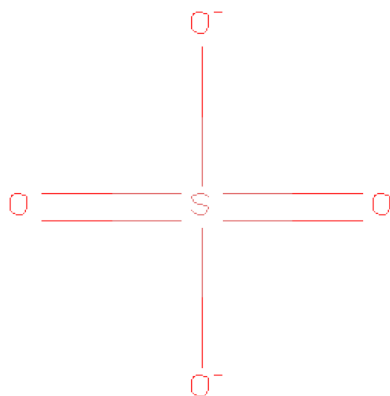
There are 3 unique types of molecules in this entry. The entry contains 3659 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENTEROTOXIN H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1708	1083	280	342	3			
1	B	212	Total	C	N	O	S	0	0	0
			1725	1089	282	351	3			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total	O	0	0
			73	73		
3	B	118	Total	O	0	0
			118	118		







## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.26Å 103.39Å 117.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40	Depositor
% Data completeness (in resolution range)	95.8 (15.00-2.40)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.214 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.40	0/1734	0.68	0/2331
1	B	0.42	0/1752	0.79	5/2357 (0.2%)
All	All	0.41	0/3486	0.74	5/4688 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	ASN	N-CA-C	-9.58	85.14	111.00
1	B	89	ILE	N-CA-C	7.97	132.52	111.00
1	B	87	GLU	N-CA-C	7.26	130.59	111.00
1	B	82	CYS	N-CA-C	-6.58	93.22	111.00
1	B	87	GLU	CA-C-N	-6.12	103.74	117.20

There are no chirality outliers.

There are no planarity outliers.

### 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	1708	0	1670	39	0
1	B	1725	0	1684	39	0
2	A	10	0	0	1	0
2	B	25	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	73	0	0	1	0
3	B	118	0	0	5	0
All	All	3659	0	3354	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 11.

All (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:A:85:ILE:HG13	1:A:85:ILE:O	1.68	0.90
1:A:85:ILE:O	1:A:86:SER:HB2	1.75	0.85
1:A:67:LYS:O	1:A:68:ASN:HB2	1.81	0.81
1:B:183:GLY:HA3	2:B:1006:SO4:O2	1.82	0.80
1:A:67:LYS:O	1:A:68:ASN:CB	2.34	0.75
1:B:88:ASN:ND2	1:B:88:ASN:O	2.19	0.71
1:B:88:ASN:HD22	1:B:88:ASN:C	1.94	0.70
1:B:115:TRP:CZ3	1:B:120:GLN:HB2	2.26	0.69
1:A:86:SER:HB3	1:A:88:ASN:N	2.08	0.69
1:A:191:LYS:O	1:A:194:GLU:HG2	1.94	0.67
1:B:167:ASP:HA	1:B:173:ASP:OD1	1.98	0.63
1:B:84:LYS:HE2	1:B:87:GLU:OE1	1.98	0.63
1:B:191:LYS:O	1:B:194:GLU:HG2	1.99	0.62
1:A:107:GLU:OE2	1:A:129:ASN:ND2	2.33	0.62
1:A:115:TRP:CZ3	1:A:120:GLN:HB2	2.36	0.61
1:B:151:LYS:HB3	1:B:154:TYR:CD2	2.34	0.61
1:A:86:SER:C	1:A:88:ASN:N	2.55	0.60
1:A:25:PHE:CZ	1:A:27:LYS:HG3	2.36	0.60
1:B:73:ILE:HG21	1:B:93:LEU:HD21	1.83	0.60
1:A:25:PHE:CE2	1:A:27:LYS:HG3	2.38	0.59
1:A:28:GLU:HG3	1:A:72:ASP:OD1	2.03	0.59
1:B:185:ASN:HB2	2:B:1006:SO4:O4	2.04	0.58
1:B:88:ASN:ND2	1:B:88:ASN:C	2.55	0.57
1:A:49:SER:HB2	1:A:51:ASN:ND2	2.19	0.57
1:B:108:ARG:NH2	1:B:204:ILE:O	2.38	0.56
1:A:89:ILE:HG12	1:A:90:SER:N	2.20	0.56
1:B:81:LYS:HG3	1:B:187:TYR:CE2	2.41	0.56
1:B:85:ILE:HG13	1:B:90:SER:HB2	1.88	0.55
1:A:30:ILE:HG22	1:A:46:GLN:HE22	1.72	0.54
1:B:151:LYS:HB3	1:B:154:TYR:HD2	1.73	0.54
1:A:69:LYS:O	1:A:71:VAL:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LEU:HD23	1:B:184:GLU:OE1	2.08	0.53
1:A:181:LEU:HB3	1:A:189:ILE:HG12	1.90	0.53
1:A:85:ILE:O	1:A:86:SER:CB	2.53	0.52
1:B:54:ARG:HB2	1:B:85:ILE:HD11	1.93	0.51
1:A:42:ILE:CG2	1:A:85:ILE:HD13	2.41	0.51
1:A:99:LEU:HD12	1:A:102:GLU:OE1	2.11	0.51
1:A:107:GLU:HG3	1:A:127:ARG:HB3	1.95	0.49
1:B:84:LYS:HG2	1:B:87:GLU:OE2	2.12	0.49
1:B:73:ILE:CG2	1:B:93:LEU:HD21	2.43	0.49
1:B:84:LYS:CE	1:B:87:GLU:OE1	2.61	0.48
1:A:35:ILE:HD13	1:A:41:LEU:HD23	1.94	0.48
1:B:109:VAL:HG22	1:B:127:ARG:HE	1.79	0.48
1:B:88:ASN:HB2	3:B:1122:HOH:O	2.14	0.48
1:B:89:ILE:N	1:B:89:ILE:HD13	2.28	0.48
1:B:174:TYR:CE2	1:B:197:LYS:HE2	2.50	0.47
1:B:89:ILE:H	1:B:89:ILE:HD13	1.79	0.47
1:B:187:TYR:CE1	1:B:188:GLU:HG2	2.50	0.47
1:A:171:PRO:HD3	1:B:212:TYR:CD2	2.49	0.47
1:A:42:ILE:HG21	1:A:85:ILE:CD1	2.44	0.47
1:B:112:ALA:HA	1:B:207:ILE:O	2.15	0.47
1:B:172:ARG:NH1	3:B:1088:HOH:O	2.47	0.47
1:A:42:ILE:HG21	1:A:85:ILE:HD13	1.98	0.46
1:B:36:SER:O	1:B:40:ASP:HB2	2.15	0.46
1:A:144:LYS:HD2	3:A:1038:HOH:O	2.14	0.45
1:B:3:LEU:HB3	3:B:1063:HOH:O	2.17	0.45
1:A:85:ILE:O	1:A:85:ILE:CG1	2.53	0.45
1:B:177:ASP:HB3	1:B:180:ASP:HB3	1.99	0.45
1:A:151:LYS:HB3	1:A:154:TYR:CD2	2.52	0.44
1:A:213:THR:O	1:A:214:LYS:CB	2.65	0.44
1:A:9:LEU:HB2	1:A:14:LEU:HD13	2.00	0.44
1:A:214:LYS:HG2	1:A:214:LYS:O	2.18	0.43
1:B:115:TRP:CE3	1:B:120:GLN:HB2	2.52	0.43
1:B:89:ILE:H	1:B:89:ILE:CD1	2.31	0.43
1:A:107:GLU:HG2	1:A:127:ARG:HD2	2.01	0.42
1:B:80:TYR:O	1:B:81:LYS:HB2	2.19	0.42
1:B:110:ILE:HD13	1:B:204:ILE:HG21	1.99	0.42
1:A:16:ASN:HB3	1:A:186:ASP:OD1	2.20	0.42
1:A:30:ILE:HG22	1:A:46:GLN:NE2	2.35	0.42
1:B:9:LEU:HA	3:B:1124:HOH:O	2.19	0.42
1:B:88:ASN:CB	3:B:1122:HOH:O	2.68	0.42
1:A:112:ALA:HA	1:A:207:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:THR:HA	1:A:198:THR:HA	2.01	0.41
1:A:77:SER:HA	1:A:92:CYS:O	2.21	0.41
1:A:213:THR:O	1:A:214:LYS:HB3	2.20	0.41
1:B:54:ARG:HD2	1:B:92:CYS:SG	2.61	0.40
1:A:128:THR:HA	2:A:1001:SO4:O2	2.22	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	208/217 (96%)	196 (94%)	12 (6%)	0	100	100
1	B	210/217 (97%)	200 (95%)	7 (3%)	3 (1%)	12	17
All	All	418/434 (96%)	396 (95%)	19 (4%)	3 (1%)	24	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	84	LYS
1	B	89	ILE
1	B	38	GLU

### 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	186/197 (94%)	175 (94%)	11 (6%)	21	34
1	B	191/197 (97%)	182 (95%)	9 (5%)	29	45
All	All	377/394 (96%)	357 (95%)	20 (5%)	25	40

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	29	ASN
1	A	61	ASP
1	A	68	ASN
1	A	74	TYR
1	A	85	ILE
1	A	86	SER
1	A	89	ILE
1	A	93	LEU
1	A	127	ARG
1	A	129	ASN
1	B	28	GLU
1	B	29	ASN
1	B	83	GLU
1	B	87	GLU
1	B	88	ASN
1	B	93	LEU
1	B	127	ARG
1	B	156	ASP
1	B	172	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	29	ASN
1	A	46	GLN
1	A	51	ASN
1	A	64	GLN
1	A	120	GLN
1	B	20	GLN
1	B	29	ASN
1	B	64	GLN
1	B	70	ASN

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Mol	Chain	Res	Type
1	B	120	GLN

### 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](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	1001	-	4,4,4	0.33	0	6,6,6	0.13	0
2	SO4	A	1005	-	4,4,4	0.30	0	6,6,6	0.08	0
2	SO4	B	1002	-	4,4,4	0.36	0	6,6,6	0.11	0
2	SO4	B	1003	-	4,4,4	0.78	0	6,6,6	0.17	0
2	SO4	B	1004	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	B	1006	-	4,4,4	0.28	0	6,6,6	0.16	0
2	SO4	B	1007	-	4,4,4	0.36	0	6,6,6	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1004	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1006	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1007	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SO4	1	0
2	B	1006	SO4	2	0

## 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.