



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:27 PM GMT

PDB ID : 1FNW  
Title : CRYSTAL STRUCTURE OF STREPTOCOCCAL PYROGENIC EXO-TOXIN A  
Authors : Earhart, C.A.; Vath, G.M.; Roggiani, M.; Schlivert, P.M.; Ohlendorf, D.H.  
Deposited on : 2000-08-23  
Resolution : 3.90 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

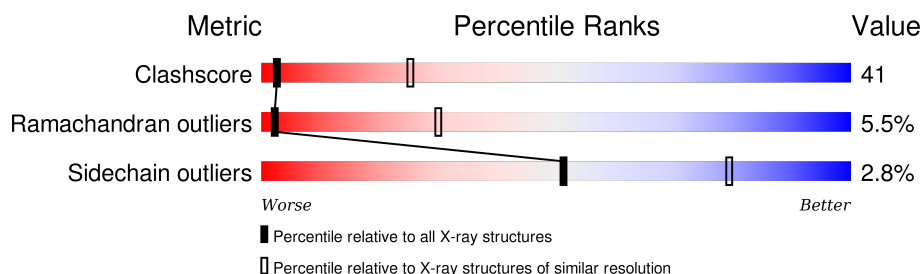
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)

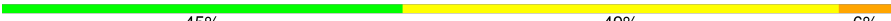
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	221	<div> <div>43%</div> <div>48%</div> <div>10%</div> </div>
1	B	221	<div> <div>44%</div> <div>50%</div> <div>6%</div> </div>
1	C	221	<div> <div>43%</div> <div>50%</div> <div>7%</div> </div>
1	D	221	<div> <div>41%</div> <div>52%</div> <div>7%</div> </div>
1	E	221	<div> <div>44%</div> <div>51%</div> <div>5%</div> </div>
1	F	221	<div> <div>44%</div> <div>51%</div> <div>5%</div> </div>
1	G	221	<div> <div>41%</div> <div>53%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	221	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: green (45%), yellow (49%), and orange (6%). The percentages are labeled below the bar. <div><div></div><div>45%</div><div>49%</div><div>6%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14616 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 EXOTOXIN TYPE A PRECURSOR (ALLELE 1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	B	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	C	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	D	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	E	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	F	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	G	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			
1	H	221	Total	C	N	O	S	0	0	0
			1823	1166	293	358	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	THR	LEU	CONFLICT	UNP P62560
A	154	ILE	THR	CONFLICT	UNP P62560
A	209	ASN	SER	CONFLICT	UNP P62560
A	210	LYS	ASN	CONFLICT	UNP P62560
B	453	THR	LEU	CONFLICT	UNP P62560
B	454	ILE	THR	CONFLICT	UNP P62560
B	509	ASN	SER	CONFLICT	UNP P62560
B	510	LYS	ASN	CONFLICT	UNP P62560
C	753	THR	LEU	CONFLICT	UNP P62560
C	754	ILE	THR	CONFLICT	UNP P62560
C	809	ASN	SER	CONFLICT	UNP P62560
C	810	LYS	ASN	CONFLICT	UNP P62560
D	1053	THR	LEU	CONFLICT	UNP P62560

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1054	ILE	THR	CONFLICT	UNP P62560
D	1109	ASN	SER	CONFLICT	UNP P62560
D	1110	LYS	ASN	CONFLICT	UNP P62560
E	1353	THR	LEU	CONFLICT	UNP P62560
E	1354	ILE	THR	CONFLICT	UNP P62560
E	1409	ASN	SER	CONFLICT	UNP P62560
E	1410	LYS	ASN	CONFLICT	UNP P62560
F	1653	THR	LEU	CONFLICT	UNP P62560
F	1654	ILE	THR	CONFLICT	UNP P62560
F	1709	ASN	SER	CONFLICT	UNP P62560
F	1710	LYS	ASN	CONFLICT	UNP P62560
G	1953	THR	LEU	CONFLICT	UNP P62560
G	1954	ILE	THR	CONFLICT	UNP P62560
G	2009	ASN	SER	CONFLICT	UNP P62560
G	2010	LYS	ASN	CONFLICT	UNP P62560
H	2253	THR	LEU	CONFLICT	UNP P62560
H	2254	ILE	THR	CONFLICT	UNP P62560
H	2309	ASN	SER	CONFLICT	UNP P62560
H	2310	LYS	ASN	CONFLICT	UNP P62560

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	4	Total Cd 4 4	0	0
2	D	4	Total Cd 4 4	0	0
2	E	4	Total Cd 4 4	0	0
2	H	3	Total Cd 3 3	0	0
2	B	4	Total Cd 4 4	0	0
2	C	4	Total Cd 4 4	0	0
2	A	4	Total Cd 4 4	0	0
2	F	5	Total Cd 5 5	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

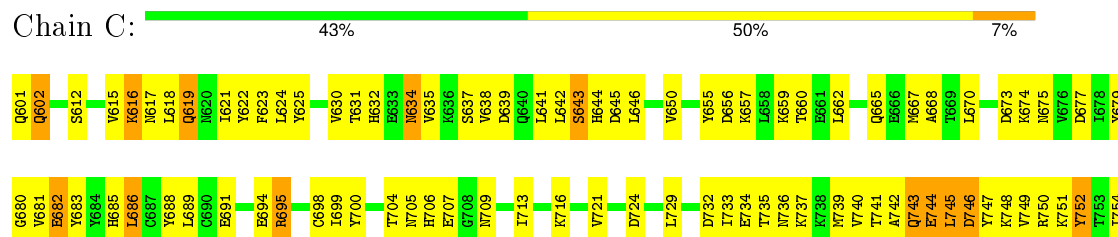
#### • Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)



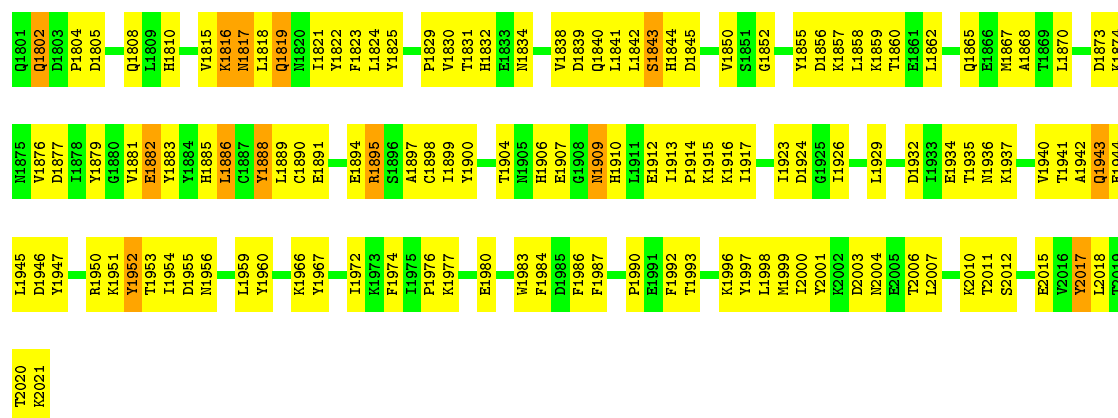
#### • Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)



#### • Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

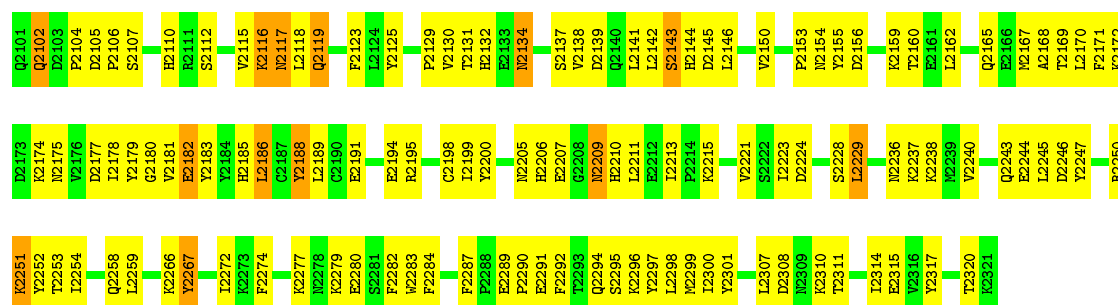






• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)

Chain H: 45% 49% 6%





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	226.23Å 226.23Å 81.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.90	Depositor
% Data completeness (in resolution range)	77.0 (20.00-3.90)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.213 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.46	0/1865	0.73	0/2522
1	B	0.46	0/1865	0.71	0/2522
1	C	0.45	0/1865	0.70	0/2522
1	D	0.45	0/1865	0.72	0/2522
1	E	0.43	0/1865	0.69	0/2522
1	F	0.46	0/1865	0.71	0/2522
1	G	0.45	0/1865	0.71	0/2522
1	H	0.45	0/1865	0.71	0/2522
All	All	0.45	0/14920	0.71	0/20176

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	1823	0	1778	157	0
1	B	1823	0	1775	151	0
1	C	1823	0	1775	149	0
1	D	1823	0	1775	159	0
1	E	1823	0	1775	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1823	0	1775	150	0
1	G	1823	0	1775	154	0
1	H	1823	0	1775	161	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	5	0	0	0	0
2	G	4	0	0	0	0
2	H	3	0	0	0	0
All	All	14616	0	14203	1180	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 41.

The worst 5 of 1180 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:619:GLN:H	1:C:619:GLN:NE2	1.55	1.03
1:B:391:GLU:HB3	1:D:991:GLU:HB3	1.36	1.03
1:H:2119:GLN:NE2	1:H:2119:GLN:H	1.54	1.03
1:E:1291:GLU:HB3	1:G:1891:GLU:HB3	1.38	1.02
1:E:1219:GLN:H	1:E:1219:GLN:NE2	1.57	1.02

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	219/221 (99%)	164 (75%)	40 (18%)	15 (7%)	<b>1</b> <b>24</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	219/221 (99%)	168 (77%)	35 (16%)	16 (7%)	1	22
1	C	219/221 (99%)	172 (78%)	34 (16%)	13 (6%)	2	28
1	D	219/221 (99%)	171 (78%)	37 (17%)	11 (5%)	3	31
1	E	219/221 (99%)	163 (74%)	46 (21%)	10 (5%)	3	33
1	F	219/221 (99%)	160 (73%)	50 (23%)	9 (4%)	3	36
1	G	219/221 (99%)	178 (81%)	31 (14%)	10 (5%)	3	33
1	H	219/221 (99%)	173 (79%)	34 (16%)	12 (6%)	2	30
All	All	1752/1768 (99%)	1349 (77%)	307 (18%)	96 (6%)	2	30

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	B	316	LYS
1	B	334	ASN
1	D	916	LYS
1	E	1216	LYS

### 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	208/208 (100%)	200 (96%)	8 (4%)	40	74
1	B	208/208 (100%)	204 (98%)	4 (2%)	65	86
1	C	208/208 (100%)	203 (98%)	5 (2%)	57	82
1	D	208/208 (100%)	200 (96%)	8 (4%)	40	74
1	E	208/208 (100%)	204 (98%)	4 (2%)	65	86
1	F	208/208 (100%)	203 (98%)	5 (2%)	57	82
1	G	208/208 (100%)	203 (98%)	5 (2%)	57	82
1	H	208/208 (100%)	201 (97%)	7 (3%)	44	77
All	All	1664/1664 (100%)	1618 (97%)	46 (3%)	51	79

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

Mol	Chain	Res	Type
1	D	988	TYR
1	E	1202	GLN
1	H	2188	TYR
1	D	1000	TYR
1	D	1090	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	908	GLN
1	E	1202	GLN
1	H	2102	GLN
1	D	919	GLN
1	D	1010	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.