



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:26 PM GMT

PDB ID : 1FNU
Title : STRUCTURE OF STREPTOCOCCAL PYROGENIC EXOTOXIN A
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Deposited on : 2000-08-23
Resolution : 1.94 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

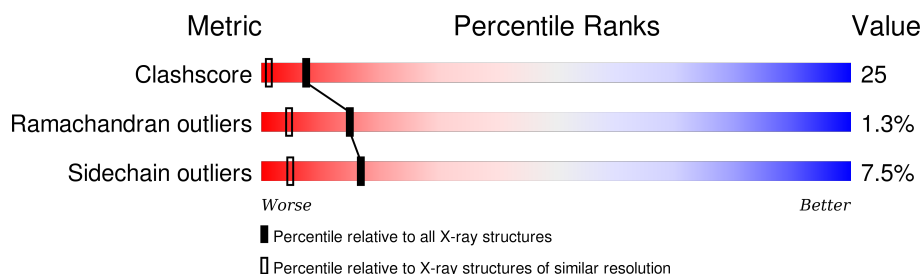
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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))
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 66% 25% 6% •
1	B	221	 73% 20% 5% •
1	C	221	 64% 30% 5%
1	D	221	 52% 39% 6% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7934 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	5	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			

There are 16 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
D	1054	ILE	THR	CONFLICT	UNP P62560
D	1109	ASN	SER	CONFLICT	UNP P62560
D	1110	LYS	ASN	CONFLICT	UNP P62560

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total 4	Cd 4	0	0
2	A	4	Total 4	Cd 4	0	0
2	D	3	Total 3	Cd 3	0	0
2	C	4	Total 4	Cd 4	0	0

- Molecule 3 is water.

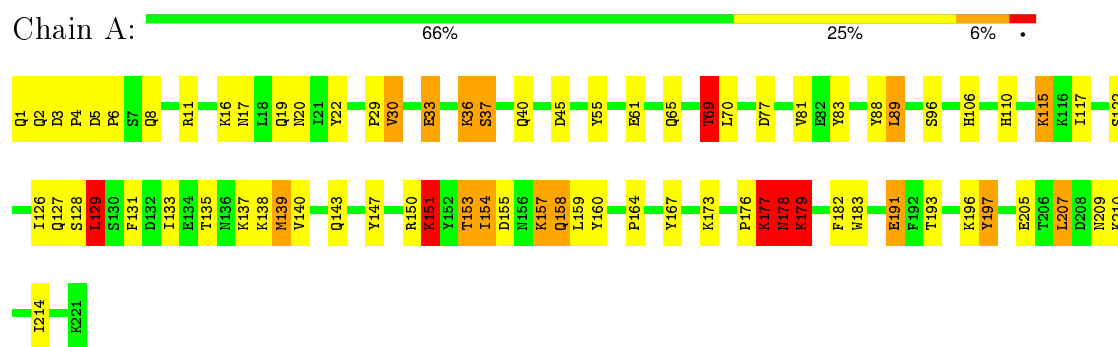
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	156	Total 156	O 156	0	0
3	B	169	Total 169	O 169	0	0
3	C	176	Total 176	O 176	0	0
3	D	126	Total 126	O 126	0	0

3 Residue-property plots

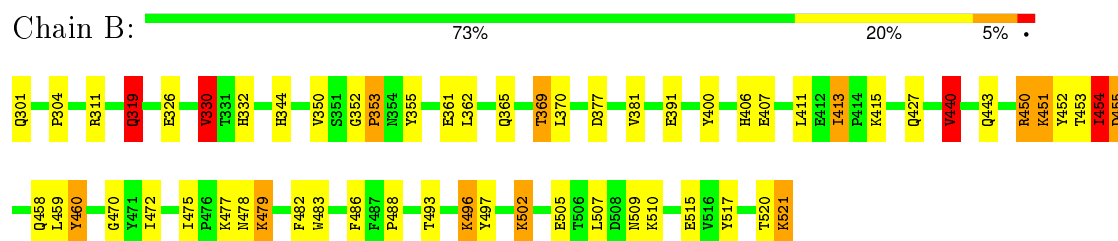
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

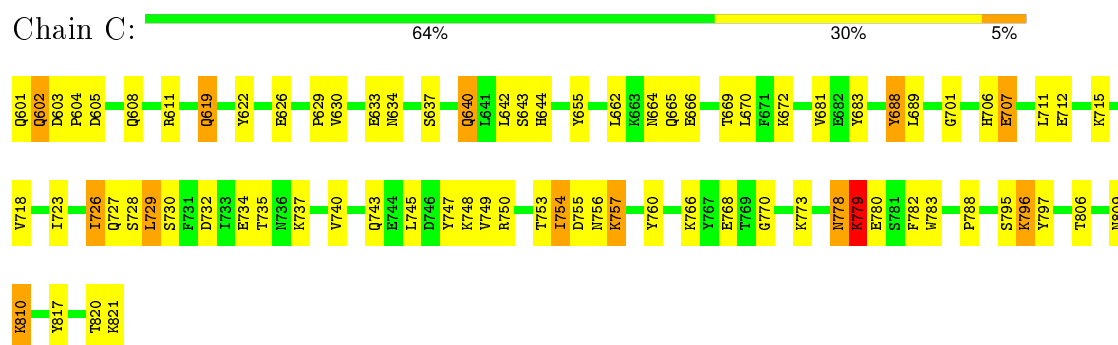
• Molecule 1: EXOTOXIN TYPE A PRECURSOR (ALLELE 1)



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

Chain D:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.30 Å 126.80 Å 148.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.94	Depositor
% Data completeness (in resolution range)	79.7 (20.00-1.94)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7934	wwPDB-VP
Average B, all atoms (Å ²)	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	1.25	7/1865 (0.4%)	1.20	8/2522 (0.3%)
1	B	1.28	8/1865 (0.4%)	1.18	12/2522 (0.5%)
1	C	1.24	4/1865 (0.2%)	1.15	7/2522 (0.3%)
1	D	1.13	2/1865 (0.1%)	1.16	8/2522 (0.3%)
All	All	1.23	21/7460 (0.3%)	1.17	35/10088 (0.3%)

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	1
1	C	0	2
1	D	0	1
All	All	0	6

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	GLN	CB-CG	7.17	1.72	1.52
1	B	452	TYR	CD1-CE1	6.96	1.49	1.39
1	C	688	TYR	CD2-CE2	6.79	1.49	1.39
1	B	502	LYS	CD-CE	6.73	1.68	1.51
1	C	688	TYR	CD1-CE1	6.38	1.49	1.39

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	VAL	CB-CA-C	-8.53	95.19	111.40
1	B	451	LYS	CD-CE-NZ	-8.02	93.26	111.70
1	B	311	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	11	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	11	ARG	NE-CZ-NH1	6.41	123.50	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	TYR	Sidechain
1	A	197	TYR	Sidechain
1	B	497	TYR	Sidechain
1	C	688	TYR	Sidechain
1	C	797	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	1823	0	1778	94	0
1	B	1823	0	1775	58	1
1	C	1823	0	1775	93	0
1	D	1823	0	1775	121	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
3	A	156	0	0	5	1
3	B	169	0	0	10	0
3	C	176	0	0	7	1
3	D	126	0	0	6	0
All	All	7934	0	7103	365	2

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 25.

The worst 5 of 365 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:605:ASP:H	1:C:608:GLN:NE2	1.35	1.22
1:B:450:ARG:O	1:B:454:ILE:HD13	1.40	1.21
1:A:1:GLN:HB2	1:A:182:PHE:HA	1.25	1.10
1:A:150:ARG:O	1:A:154:ILE:HD13	1.48	1.10
1:C:723:ILE:O	1:C:726:ILE:HD13	1.56	1.05

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2128:HOH:O	3:A:3010:HOH:O[1_655]	1.69	0.51
1:B:455:ASP:O	3:C:5073:HOH:O[3_545]	2.18	0.02

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	219/221 (99%)	206 (94%)	9 (4%)	4 (2%)	11	2
1	B	219/221 (99%)	208 (95%)	11 (5%)	0	100	100
1	C	219/221 (99%)	211 (96%)	6 (3%)	2 (1%)	21	9
1	D	219/221 (99%)	195 (89%)	19 (9%)	5 (2%)	8	1
All	All	876/884 (99%)	820 (94%)	45 (5%)	11 (1%)	15	5

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	727	GLN
1	D	907	SER
1	D	1112	SER
1	A	178	ASN
1	C	729	LEU

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	208/208 (100%)	190 (91%)	18 (9%)	13	3
1	B	208/208 (100%)	195 (94%)	13 (6%)	22	8
1	C	208/208 (100%)	199 (96%)	9 (4%)	35	19
1	D	208/208 (100%)	186 (89%)	22 (11%)	8	1
All	All	832/832 (100%)	770 (92%)	62 (8%)	17	5

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	488	PRO
1	C	726	ILE
1	D	1079	LYS
1	C	602	GLN
1	C	778	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	443	GLN
1	C	608	GLN
1	D	1058	GLN
1	B	458	GLN
1	C	601	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](#)

Of 15 ligands modelled in this entry, 15 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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