



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:32 PM GMT

PDB ID : 1G24
Title : THE CRYSTAL STRUCTURE OF EXOENZYME C3 FROM CLOSTRIDIUM BOTULINUM
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Deposited on : 2000-10-16
Resolution : 1.70 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

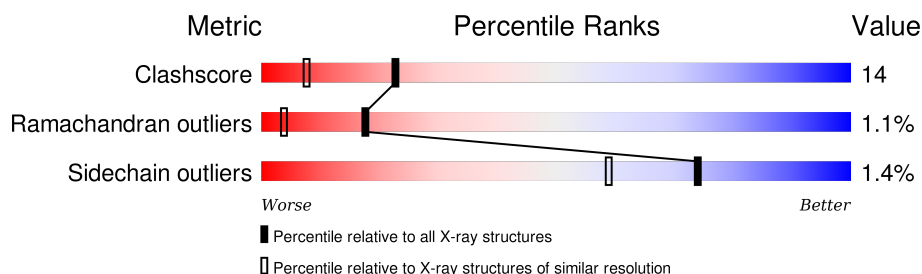
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)

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	211	<div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	B	211	<div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	C	211	<div> <div>71%</div> <div>28%</div> </div>
1	D	211	<div> <div>74%</div> <div>25%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7493 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 EXOENZYME C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1656	1053	282	314	7			
1	B	211	Total	C	N	O	S	0	0	0
			1656	1053	282	314	7			
1	C	211	Total	C	N	O	S	0	0	0
			1656	1053	282	314	7			
1	D	211	Total	C	N	O	S	0	0	0
			1656	1053	282	314	7			

- Molecule 2 is water.

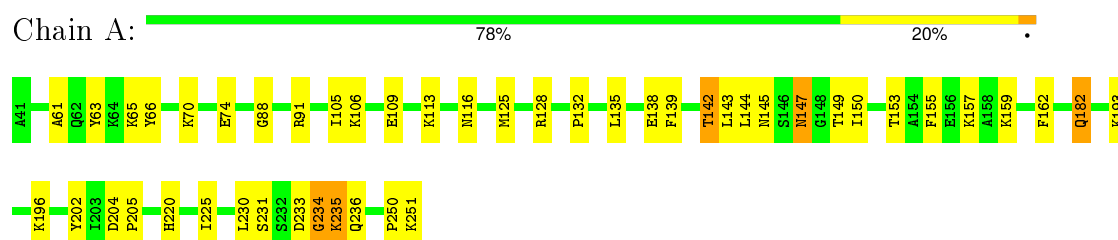
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	202	Total	O	0	0
			202	202		
2	B	224	Total	O	0	0
			224	224		
2	C	221	Total	O	0	0
			221	221		
2	D	222	Total	O	0	0
			222	222		

3 Residue-property plots

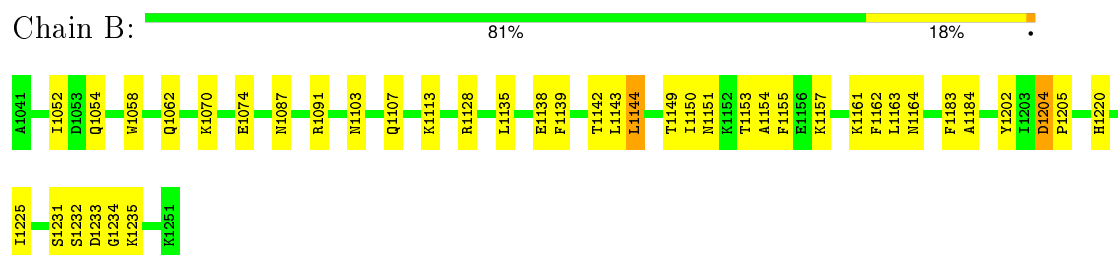
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

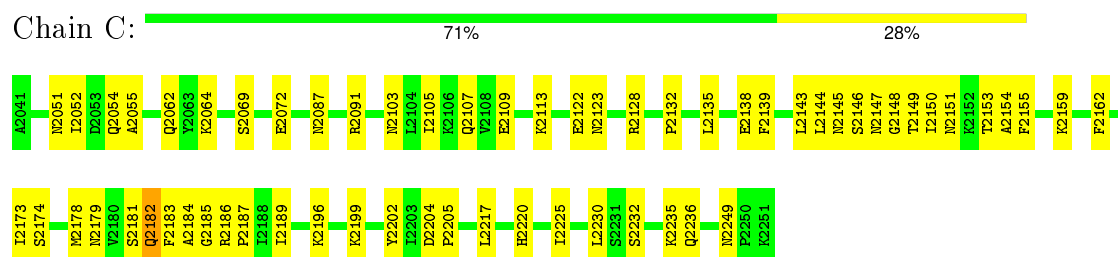
• Molecule 1: EXOENZYME C3



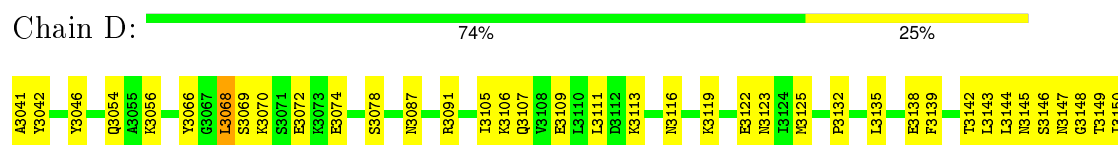
• Molecule 1: EXOENZYME C3



• Molecule 1: EXOENZYME C3



• Molecule 1: EXOENZYME C3



N3151	K3152	T3153	A3154	F3155	K3159	F3162	Y3172	Q3182	K3193	K3196	L3213	I3225	L3230	K3235	Q3236	I3237	K3251
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4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	233.75Å 73.76Å 73.75Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70	Depositor
% Data completeness (in resolution range)	9.4 (30.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	5.70	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7493	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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	0.30	0/1686	0.58	0/2266
1	B	0.31	0/1686	0.58	0/2266
1	C	0.32	0/1686	0.59	0/2266
1	D	0.31	0/1686	0.57	0/2266
All	All	0.31	0/6744	0.58	0/9064

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	1656	0	1677	43	0
1	B	1656	0	1677	28	0
1	C	1656	0	1677	66	0
1	D	1656	0	1677	44	0
2	A	202	0	0	3	0
2	B	224	0	0	1	0
2	C	221	0	0	6	0
2	D	222	0	0	5	0
All	All	7493	0	6708	181	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 14.

The worst 5 of 181 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:2052:ILE:HA	1:C:2178:MET:HE1	1.29	1.14
1:A:135:LEU:HD12	1:A:143:LEU:HD11	1.43	0.99
1:A:149:THR:HB	1:A:235:LYS:HD2	1.44	0.97
1:C:2150:ILE:HG12	1:C:2235:LYS:HB3	1.53	0.89
1:A:150:ILE:HG12	1:A:235:LYS:HB3	1.55	0.86

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	209/211 (99%)	197 (94%)	7 (3%)	5 (2%)	7	1
1	B	209/211 (99%)	200 (96%)	7 (3%)	2 (1%)	19	4
1	C	209/211 (99%)	199 (95%)	9 (4%)	1 (0%)	34	15
1	D	209/211 (99%)	197 (94%)	11 (5%)	1 (0%)	34	15
All	All	836/844 (99%)	793 (95%)	34 (4%)	9 (1%)	17	4

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	B	1184	ALA
1	C	2182	GLN
1	A	233	ASP
1	B	1144	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	179/179 (100%)	175 (98%)	4 (2%)	60	39
1	B	179/179 (100%)	177 (99%)	2 (1%)	80	69
1	C	179/179 (100%)	177 (99%)	2 (1%)	80	69
1	D	179/179 (100%)	177 (99%)	2 (1%)	80	69
All	All	716/716 (100%)	706 (99%)	10 (1%)	74	59

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1204	ASP
1	B	1220	HIS
1	C	2220	HIS
1	A	220	HIS
1	C	2051	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2140	GLN
1	C	2164	ASN
1	D	3151	ASN
1	C	2151	ASN
1	C	2182	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](#)

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 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.