



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:22 am GMT

PDB ID : 1CLX
Title : CATALYTIC CORE OF XYLANASE A
Authors : Harris, G.W.; Jenkins, J.A.; Connerton, I.; Pickersgill, R.W.
Deposited on : 1995-08-31
Resolution : 1.80 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

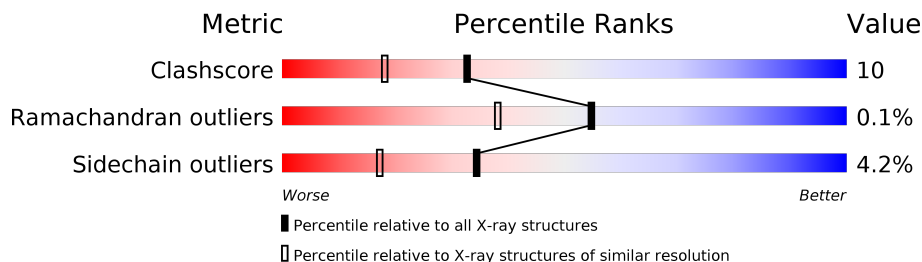
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)

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	347	
1	B	347	
1	C	347	
1	D	347	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11908 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 XYLANASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2699	1693	479	519	8			
1	B	345	Total	C	N	O	S	0	0	0
			2699	1693	479	519	8			
1	C	345	Total	C	N	O	S	0	0	0
			2699	1693	479	519	8			
1	D	345	Total	C	N	O	S	0	0	0
			2699	1693	479	519	8			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		


- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	272	Total	O	0	0
			272	272		
3	B	278	Total	O	0	0
			278	278		
3	C	276	Total	O	0	0
			276	276		
3	D	282	Total	O	0	0
			282	282		

Note EDS was not executed.

- Chain A:
-
- 74% 20%
- Chain A: R146, R147, S148, V149, F150, Y151, R152, Q153, F154, G155, G156, Y159, I160, D161, E162, R165, R166, A167, R168, T173, A174, E175, Y178, V194, R195, L196, Y197, Q198, R199, V205, M217, R218, D219, Y220, T223, R227, W230, S237, P238, T239, L240, V249, R250, D256, R258, R282, Y283, K284, Y290, V294, P295, P296, A308, D309, Y315, T316, R317, Q318, D322, D329, R330, L331, V341, E342, S345, GLY, ARG

- Chain B:

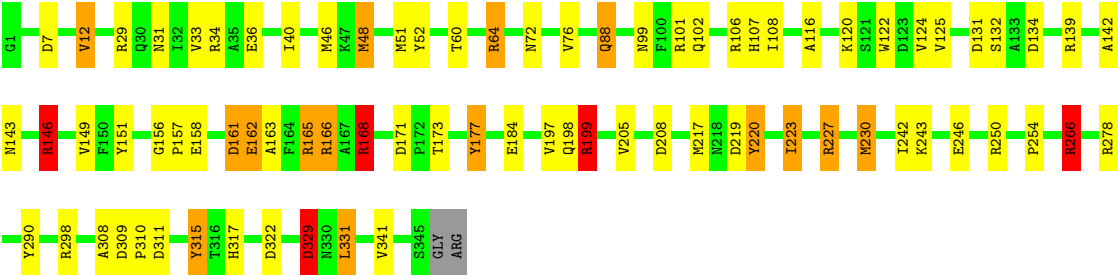
- Chain C: 

● Molecule 1: XYLANASE A

Chain D:

76%

17%



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, α , β , γ	96.11Å 97.32Å 151.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11908	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: CA

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	0.90	0/2766	1.54	39/3769 (1.0%)
1	B	0.92	0/2766	1.48	33/3769 (0.9%)
1	C	0.92	1/2766 (0.0%)	1.49	39/3769 (1.0%)
1	D	0.91	0/2766	1.52	46/3769 (1.2%)
All	All	0.91	1/11064 (0.0%)	1.51	157/15076 (1.0%)

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	8
1	B	0	7
1	C	0	12
1	D	0	8
All	All	0	35

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	313	TRP	NE1-CE2	-5.07	1.30	1.37

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ARG	NE-CZ-NH1	16.88	128.74	120.30
1	B	146	ARG	NE-CZ-NH1	15.60	128.10	120.30
1	D	266	ARG	NE-CZ-NH1	14.60	127.60	120.30
1	D	266	ARG	CD-NE-CZ	14.28	143.59	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	266	ARG	NE-CZ-NH2	-14.24	113.18	120.30

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	TRP	Peptide
1	A	146	ARG	Sidechain
1	A	152	ARG	Sidechain
1	A	166	ARG	Sidechain
1	A	64	ARG	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	2699	0	2560	52	6
1	B	2699	0	2560	46	2
1	C	2699	0	2560	61	1
1	D	2699	0	2560	50	4
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	272	0	0	13	9
3	B	278	0	0	10	3
3	C	276	0	0	16	3
3	D	282	0	0	17	10
All	All	11908	0	10240	209	20

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 10.

The worst 5 of 209 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:143:ASN:CG	3:C:1031:HOH:O	1.77	1.20
1:C:198:GLN:CG	3:C:1123:HOH:O	1.99	1.09
1:C:198:GLN:HG3	3:C:1123:HOH:O	1.53	1.08
1:C:161:ASP:OD1	1:C:199:ARG:NH2	1.92	1.00
1:C:61:ASN:HD22	1:C:64:ARG:HH12	1.08	0.99

The worst 5 of 20 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:622:HOH:O	3:D:1395:HOH:O[2_675]	0.78	1.42
3:A:477:HOH:O	3:A:546:HOH:O[3_646]	0.88	1.32
3:A:507:HOH:O	3:D:1354:HOH:O[3_656]	1.28	0.92
3:B:899:HOH:O	3:D:1286:HOH:O[3_656]	1.40	0.80
3:A:547:HOH:O	3:A:597:HOH:O[3_656]	1.47	0.73

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	343/347 (99%)	331 (96%)	11 (3%)	1 (0%)	44	29
1	B	343/347 (99%)	332 (97%)	11 (3%)	0	100	100
1	C	343/347 (99%)	332 (97%)	11 (3%)	0	100	100
1	D	343/347 (99%)	330 (96%)	13 (4%)	0	100	100
All	All	1372/1388 (99%)	1325 (97%)	46 (3%)	1 (0%)	55	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	GLY

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	283/284 (100%)	271 (96%)	12 (4%)	34	17
1	B	283/284 (100%)	269 (95%)	14 (5%)	29	12
1	C	283/284 (100%)	273 (96%)	10 (4%)	41	24
1	D	283/284 (100%)	271 (96%)	12 (4%)	34	17
All	All	1132/1136 (100%)	1084 (96%)	48 (4%)	34	17

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	166	ARG
1	C	25	THR
1	D	227	ARG
1	B	168	ARG
1	B	223	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	203	ASN
1	C	61	ASN
1	D	317	HIS
1	B	319	ASN
1	A	203	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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.