



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2019 – 10:38 PM EDT

PDB ID : 6UJE
Title : Crystal structure of the Clostridial cellulose synthase subunit Z (CcsZ) from Clostridioides difficile
Deposited on : 2019-10-03
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at 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.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

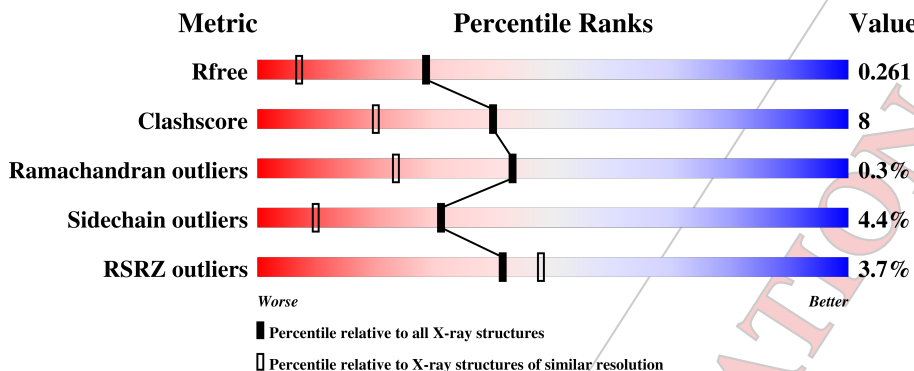
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.5
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.5

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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))
R_{free}	111664	1952 (1.76-1.76)
Clashscore	122126	2072 (1.76-1.76)
Ramachandran outliers	120053	2050 (1.76-1.76)
Sidechain outliers	120020	2050 (1.76-1.76)
RSRZ outliers	108989	1913 (1.76-1.76)

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.

Mol	Chain	Length	Quality of chain
1	A	320	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2763 atoms, of which 86 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 Endoglucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	301	2642	1656	86	422	474	4	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	initiating methionine	UNP A0A449M8I9
A	41	LYS	GLN	conflict	UNP A0A449M8I9
A	99	ASP	GLU	conflict	UNP A0A449M8I9
A	274	ASN	LYS	conflict	UNP A0A449M8I9
A	343	LEU	-	expression tag	UNP A0A449M8I9
A	344	GLU	-	expression tag	UNP A0A449M8I9
A	345	HIS	-	expression tag	UNP A0A449M8I9
A	346	HIS	-	expression tag	UNP A0A449M8I9
A	347	HIS	-	expression tag	UNP A0A449M8I9
A	348	HIS	-	expression tag	UNP A0A449M8I9
A	349	HIS	-	expression tag	UNP A0A449M8I9
A	350	HIS	-	expression tag	UNP A0A449M8I9

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

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

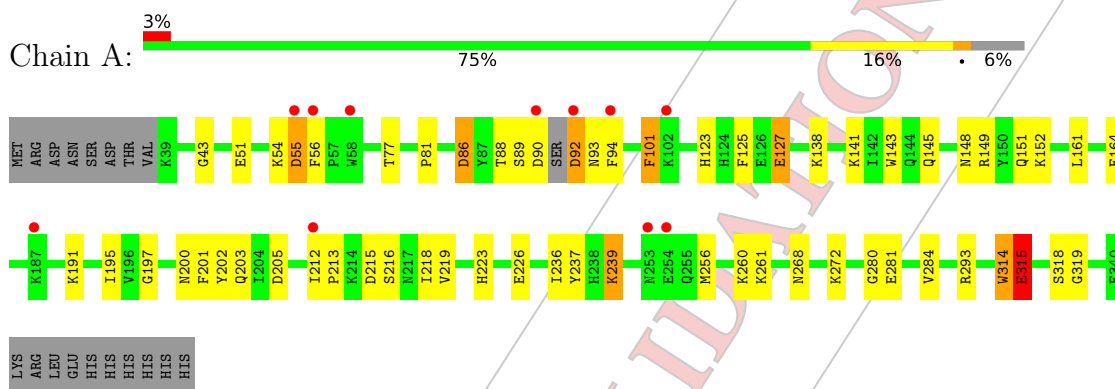
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	0	0
			120	120		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

- Molecule 1: Endoglucanase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.95Å 45.63Å 59.94Å 90.00° 94.99° 90.00°	Depositor
Resolution (Å)	43.04 – 1.75 43.04 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.9 (43.04-1.75) 96.9 (43.04-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.75Å)	Xtrriage
Refinement program	PHENIX 1.14 3260	Depositor
R, R_{free}	0.227 , 0.260 0.236 , 0.261	Depositor DCC
R_{free} test set	1508 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtrriage
Anisotropy	0.339	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2763	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.44	5/2626 (0.2%)	0.57	6/3544 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	GLU	C-N	7.74	1.49	1.34
1	A	127	GLU	CD-OE2	-6.95	1.18	1.25
1	A	226	GLU	CD-OE2	-6.37	1.18	1.25
1	A	226	GLU	CD-OE1	-5.85	1.19	1.25
1	A	315	GLU	CD-OE1	-5.54	1.19	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	GLU	CB-CA-C	11.03	132.46	110.40
1	A	315	GLU	CB-CG-CD	-9.01	89.88	114.20
1	A	314	TRP	O-C-N	6.78	133.54	122.70
1	A	315	GLU	N-CA-CB	-6.13	99.56	110.60
1	A	314	TRP	N-CA-CB	6.08	121.53	110.60
1	A	314	TRP	CA-C-N	-5.19	105.78	117.20

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	2556	86	2483	40	1
2	A	1	0	0	0	0
3	A	120	0	0	2	0
All	All	2677	86	2483	40	1

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 8.

All (40) 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:215:ASP:HB3	1:A:218:ILE:HD12	1.53	0.91
1:A:239:LYS:NZ	1:A:239:LYS:HB3	1.94	0.81
1:A:236:ILE:HD12	1:A:237:TYR:N	2.05	0.70
1:A:239:LYS:HZ2	1:A:239:LYS:HB3	1.57	0.70
1:A:212:ILE:HD12	1:A:212:ILE:H	1.59	0.68
1:A:101:PHE:CZ	1:A:149:ARG:HD3	2.37	0.60
1:A:213:PRO:HG2	1:A:218:ILE:HD13	1.85	0.59
1:A:268:ASN:O	1:A:272:LYS:HG3	2.03	0.59
1:A:215:ASP:HB3	1:A:218:ILE:CD1	2.30	0.58
1:A:200:ASN:O	1:A:203:GLN:HB2	2.04	0.57
1:A:101:PHE:CE1	1:A:149:ARG:HD3	2.41	0.56
1:A:43:GLY:HA2	1:A:77:THR:O	2.09	0.52
1:A:197:GLY:HA3	1:A:202:TYR:CE1	2.44	0.52
1:A:164:GLU:HB3	1:A:201:PHE:HA	1.92	0.51
1:A:195:ILE:HG12	1:A:219:VAL:HB	1.93	0.51
1:A:223:HIS:CG	1:A:281:GLU:HB2	2.46	0.51
1:A:236:ILE:HD11	1:A:237:TYR:CE2	2.46	0.51
1:A:151:GLN:HG3	1:A:152:LYS:HD3	1.93	0.51
1:A:314:TRP:CD2	1:A:315:GLU:HB2	2.47	0.50
1:A:143:TRP:CZ2	1:A:161:LEU:HA	2.47	0.49
1:A:92:ASP:N	1:A:92:ASP:OD1	2.45	0.49
1:A:212:ILE:HD12	1:A:212:ILE:N	2.28	0.49
1:A:236:ILE:HD12	1:A:237:TYR:H	1.76	0.49
1:A:261:LYS:O	1:A:261:LYS:HD2	2.13	0.49
1:A:195:ILE:HA	1:A:219:VAL:O	2.14	0.48
1:A:94:PHE:O	1:A:145:GLN:NE2	2.40	0.46
1:A:54:LYS:HE2	1:A:86:ASP:O	2.15	0.46
1:A:81:PRO:HB3	1:A:123:HIS:CG	2.52	0.45
1:A:89:SER:OG	1:A:94:PHE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:THR:OG1	1:A:138:LYS:HE3	2.18	0.44
1:A:51:GLU:HB3	1:A:81:PRO:HB2	2.00	0.43
1:A:213:PRO:CG	1:A:218:ILE:HD13	2.48	0.43
1:A:89:SER:O	1:A:94:PHE:HA	2.18	0.43
1:A:284:VAL:HB	1:A:293:ARG:HG3	2.01	0.43
1:A:148:ASN:O	1:A:151:GLN:HG2	2.20	0.42
1:A:280:GLY:HA3	3:A:519:HOH:O	2.19	0.42
1:A:256:MET:O	1:A:260:LYS:HG3	2.20	0.42
1:A:141:LYS:O	1:A:145:GLN:HG3	2.20	0.41
1:A:315:GLU:CD	1:A:318:SER:HB3	2.41	0.41
1:A:319:GLY:HA3	3:A:560:HOH:O	2.19	0.41

All (1) 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)
1:A:55:ASP:O	1:A:93:ASN:ND2[2_546]	2.18	0.02

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	298/320 (93%)	284 (95%)	13 (4%)	1 (0%)	43 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	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	276/294 (94%)	264 (96%)	12 (4%)	32 10

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	56	PHE
1	A	86	ASP
1	A	90	ASP
1	A	92	ASP
1	A	101	PHE
1	A	125	PHE
1	A	127	GLU
1	A	191	LYS
1	A	205	ASP
1	A	216	SER
1	A	239	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 1 ligands modelled in this entry, 1 is 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.

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6 Fit of model and data [i](#)

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	301/320 (94%)	0.59	11 (3%) 41 48	28, 43, 59, 74	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	PHE	4.1
1	A	90	ASP	3.1
1	A	58	TRP	3.0
1	A	92	ASP	2.9
1	A	94	PHE	2.4
1	A	187	LYS	2.4
1	A	102	LYS	2.2
1	A	254	GLU	2.1
1	A	55	ASP	2.1
1	A	212	ILE	2.1
1	A	253	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	401	1/1	0.95	0.43	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.

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