



# Full wwPDB X-ray Structure Validation Report ⓘ

May 9, 2023 – 10:25 pm BST

PDB ID : 8A14  
Title : Crystal structure of the cerato-platanin-like protein Cpl1 from *Ustilago maydis*  
Authors : Weiland, P.; Bange, G.; Altegoer, F.  
Deposited on : 2022-05-31  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.32.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.2

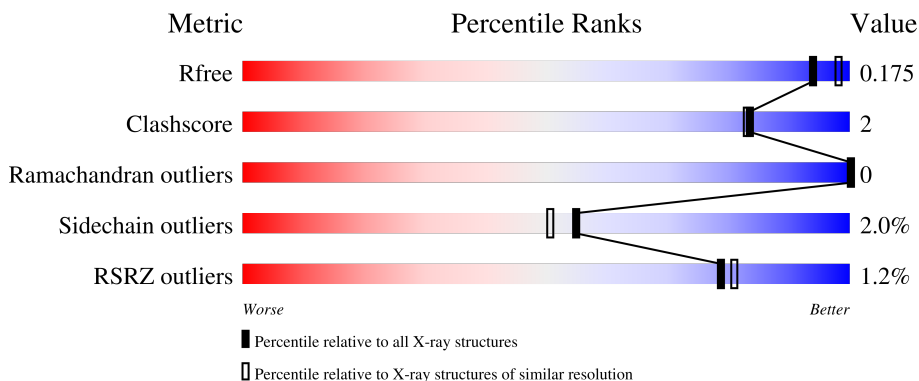
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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.



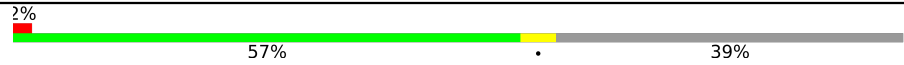
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	324	
1	B	324	
1	C	324	
1	D	324	
1	E	324	

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Mol	Chain	Length	Quality of chain
1	F	324	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '57%', and a grey segment at the end labeled '39%'. A small black dot is visible on the green segment.</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11215 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 Cerato-platanin-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	198	Total 1619	C 1043	N 269	O 299	S 8	0	0	0
1	B	198	Total 1619	C 1043	N 269	O 299	S 8	0	0	0
1	C	198	Total 1619	C 1043	N 269	O 299	S 8	0	0	0
1	D	198	Total 1619	C 1043	N 269	O 299	S 8	0	0	0
1	E	198	Total 1619	C 1043	N 269	O 299	S 8	0	0	0
1	F	198	Total 1619	C 1043	N 269	O 299	S 8	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	255	Total 255	O 255	0	0
2	B	262	Total 262	O 262	0	0
2	C	244	Total 244	O 244	0	0
2	D	259	Total 259	O 259	0	0
2	E	243	Total 243	O 243	0	0
2	F	238	Total 238	O 238	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.25Å 121.92Å 181.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.84 – 1.90 49.37 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.84-1.90) 100.0 (49.37-1.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.149 , 0.177 0.148 , 0.175	Depositor DCC
$R_{free}$ test set	7449 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtrriage
Anisotropy	0.246	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

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	0.82	0/1671	0.80	2/2267 (0.1%)
1	B	0.84	1/1671 (0.1%)	0.79	2/2267 (0.1%)
1	C	0.90	3/1671 (0.2%)	0.79	1/2267 (0.0%)
1	D	0.80	0/1671	0.81	3/2267 (0.1%)
1	E	0.87	2/1671 (0.1%)	0.78	0/2267
1	F	0.78	0/1671	0.80	3/2267 (0.1%)
All	All	0.84	6/10026 (0.1%)	0.80	11/13602 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	211	GLU	CG-CD	9.11	1.65	1.51
1	C	211	GLU	CB-CG	8.64	1.68	1.52
1	B	71	LYS	CE-NZ	6.63	1.65	1.49
1	E	72	GLU	CD-OE2	6.24	1.32	1.25
1	C	71	LYS	CE-NZ	6.07	1.64	1.49
1	E	72	GLU	CD-OE1	5.28	1.31	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	139	LYS	CD-CE-NZ	-7.21	95.11	111.70
1	D	191	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	C	189	ASP	CB-CG-OD1	6.43	124.09	118.30
1	D	222	ASP	CB-CG-OD1	6.26	123.94	118.30
1	F	162	MET	CG-SD-CE	-6.11	90.43	100.20
1	B	91	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	69	ASP	CB-CG-OD1	5.26	123.04	118.30
1	F	83	ALA	C-N-CA	-5.21	111.35	122.30
1	A	91	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	240	GLY	CA-C-O	-5.09	111.44	120.60
1	A	222	ASP	CB-CG-OD1	5.06	122.86	118.30



There are no chirality outliers.

There are no planarity outliers.

## 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	1619	0	1539	11	0
1	B	1619	0	1539	12	0
1	C	1619	0	1539	6	0
1	D	1619	0	1539	5	0
1	E	1619	0	1539	9	0
1	F	1619	0	1539	4	0
2	A	255	0	0	1	0
2	B	262	0	0	1	0
2	C	244	0	0	2	0
2	D	259	0	0	1	0
2	E	243	0	0	1	0
2	F	238	0	0	0	0
All	All	11215	0	9234	46	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 2.

All (46) 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:114:LYS:HE3	1:A:116:GLU:H	1.35	0.91
1:B:55:GLN:HE22	1:B:59:ARG:HH21	1.36	0.73
1:C:139:LYS:HD3	1:C:140:TYR:CE2	2.23	0.73
1:D:69:ASP:OD1	1:D:71:LYS:HG2	1.92	0.69
1:A:114:LYS:NZ	2:A:301:HOH:O	2.27	0.68
1:C:43:GLN:N	2:C:301:HOH:O	2.27	0.67
1:A:167:LYS:NZ	1:A:172:GLU:OE2	2.28	0.65
1:A:114:LYS:HE3	1:A:116:GLU:N	2.11	0.62
1:C:132:GLN:NE2	2:C:304:HOH:O	2.36	0.59
1:B:139:LYS:H	1:B:139:LYS:CE	2.17	0.57
1:A:54:ASN:HB3	1:A:58:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:GLU:HG2	1:F:216:LYS:HG2	1.88	0.56
1:A:114:LYS:CE	1:A:116:GLU:H	2.15	0.55
1:B:139:LYS:H	1:B:139:LYS:CD	2.23	0.52
1:C:140:TYR:HD1	1:C:209:MET:HG2	1.75	0.50
1:F:215:ASP:HB2	1:F:218:LYS:HD2	1.94	0.50
1:E:139:LYS:HG3	1:E:140:TYR:CE2	2.48	0.49
1:D:139:LYS:HD3	1:D:140:TYR:CE2	2.48	0.48
1:B:139:LYS:H	1:B:139:LYS:HE2	1.78	0.48
1:A:72:GLU:HB3	1:D:190:LYS:HB3	1.98	0.46
1:A:114:LYS:HA	1:A:114:LYS:HD2	1.67	0.46
1:B:55:GLN:NE2	1:B:59:ARG:HH21	2.10	0.46
1:C:50:MET:O	1:C:50:MET:HG3	2.16	0.46
1:E:70:VAL:HA	1:E:104:PHE:HB3	1.97	0.45
1:A:139:LYS:HG2	1:A:140:TYR:CE2	2.52	0.44
1:B:188:TRP:HB3	1:B:194:GLU:HG2	2.00	0.44
1:D:66:PRO:HA	2:D:401:HOH:O	2.18	0.43
1:E:220:VAL:HG21	1:E:225:LYS:HD3	1.99	0.43
1:E:50:MET:HG2	1:E:51:ASN:N	2.33	0.43
1:B:79:TRP:CD2	1:B:199:PRO:HA	2.53	0.43
1:B:139:LYS:HE2	2:B:436:HOH:O	2.19	0.43
1:F:79:TRP:CD2	1:F:199:PRO:HA	2.53	0.43
1:C:79:TRP:CD2	1:C:199:PRO:HA	2.54	0.43
1:F:70:VAL:HA	1:F:104:PHE:HB3	2.01	0.42
1:B:193:LYS:HB3	1:B:193:LYS:HE3	1.82	0.42
1:E:71:LYS:NZ	2:E:306:HOH:O	2.52	0.42
1:B:50:MET:HG2	1:B:51:ASN:N	2.35	0.41
1:E:44:LYS:HE3	1:E:44:LYS:HB2	1.57	0.41
1:E:79:TRP:CZ2	1:E:86:PHE:HB3	2.56	0.41
1:A:71:LYS:HD3	1:A:71:LYS:HA	1.79	0.41
1:B:126:ASP:OD1	1:B:126:ASP:N	2.49	0.41
1:B:139:LYS:H	1:B:139:LYS:HD3	1.86	0.41
1:A:114:LYS:HG3	1:A:117:PRO:CD	2.52	0.40
1:E:79:TRP:CD2	1:E:199:PRO:HA	2.55	0.40
1:E:209:MET:HE2	1:E:209:MET:HB2	1.91	0.40
1:D:209:MET:HE2	1:D:209:MET:HB2	1.93	0.40

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	196/324 (60%)	192 (98%)	4 (2%)	0	100	100
1	B	196/324 (60%)	192 (98%)	4 (2%)	0	100	100
1	C	196/324 (60%)	192 (98%)	4 (2%)	0	100	100
1	D	196/324 (60%)	192 (98%)	4 (2%)	0	100	100
1	E	196/324 (60%)	193 (98%)	3 (2%)	0	100	100
1	F	196/324 (60%)	191 (97%)	5 (3%)	0	100	100
All	All	1176/1944 (60%)	1152 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	172/275 (62%)	168 (98%)	4 (2%)	50	45
1	B	172/275 (62%)	169 (98%)	3 (2%)	60	57
1	C	172/275 (62%)	168 (98%)	4 (2%)	50	45
1	D	172/275 (62%)	168 (98%)	4 (2%)	50	45
1	E	172/275 (62%)	169 (98%)	3 (2%)	60	57
1	F	172/275 (62%)	169 (98%)	3 (2%)	60	57
All	All	1032/1650 (62%)	1011 (98%)	21 (2%)	55	51

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	TYR
1	A	114	LYS
1	A	149	MET
1	A	173	GLU
1	B	74	TYR
1	B	149	MET
1	B	190	LYS
1	C	50	MET
1	C	74	TYR
1	C	113	PHE
1	C	149	MET
1	D	74	TYR
1	D	149	MET
1	D	174	LYS
1	D	209	MET
1	E	74	TYR
1	E	149	MET
1	E	209	MET
1	F	74	TYR
1	F	85	SER
1	F	149	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	B	55	GLN
1	B	212	GLN
1	C	132	GLN
1	F	212	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 monosaccharides 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	198/324 (61%)	-0.27	0 <b>100</b> <b>100</b>	20, 28, 45, 64	0
1	B	198/324 (61%)	-0.45	1 (0%) <b>91</b> <b>92</b>	20, 29, 47, 64	0
1	C	198/324 (61%)	-0.48	1 (0%) <b>91</b> <b>92</b>	20, 29, 46, 61	0
1	D	198/324 (61%)	-0.23	3 (1%) <b>73</b> <b>76</b>	19, 28, 45, 63	0
1	E	198/324 (61%)	-0.44	2 (1%) <b>82</b> <b>84</b>	20, 28, 47, 64	0
1	F	198/324 (61%)	-0.24	7 (3%) <b>44</b> <b>47</b>	20, 29, 56, 72	0
All	All	1188/1944 (61%)	-0.35	14 (1%) <b>79</b> <b>81</b>	19, 29, 47, 72	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	217	ASN	3.8
1	B	217	ASN	3.2
1	F	43	GLN	2.8
1	F	223	TYR	2.5
1	D	135	GLU	2.4
1	C	217	ASN	2.3
1	F	224	SER	2.2
1	E	196	ASP	2.1
1	F	221	PRO	2.1
1	D	136	GLY	2.1
1	F	218	LYS	2.1
1	E	193	LYS	2.0
1	D	125	PHE	2.0
1	F	214	PHE	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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.