



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2018 – 07:41 pm GMT

PDB ID : 2V8I  
Title : Structure of a Family 2 Pectate Lyase in a Native Form  
Authors : Abbott, D.W.; Boraston, A.B.  
Deposited on : 2007-08-08  
Resolution : 1.50 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.

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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 : trunk30967  
Percentile statistics : (not set)  
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) : trunk30967

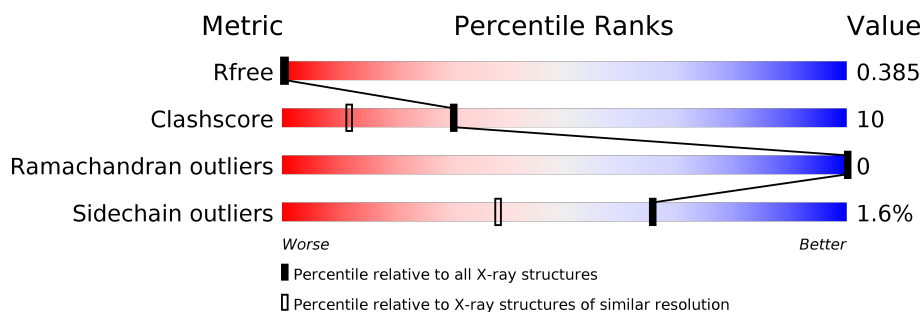
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2534 (1.50-1.50)
Clashscore	122126	2727 (1.50-1.50)
Ramachandran outliers	120053	2661 (1.50-1.50)
Sidechain outliers	120020	2659 (1.50-1.50)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	543	 89%                      11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	1547	-	-	X	-
2	IOD	A	1549	-	-	X	-
2	IOD	A	1552	-	-	X	-
2	IOD	A	1554	-	-	X	-
2	IOD	A	1555	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	1560	-	-	X	-
2	IOD	A	1563	-	-	X	-
2	IOD	A	1564	-	-	X	-
2	IOD	A	1567	-	-	X	-
2	IOD	A	1568	-	-	X	-
2	IOD	A	1569	-	-	X	-
2	IOD	A	1572	-	-	X	-
2	IOD	A	1573	-	-	X	-
2	IOD	A	1576	-	-	X	-
2	IOD	A	1588	-	-	X	-
2	IOD	A	1589	-	-	X	-
2	IOD	A	1592	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5172 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 PECTATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	5	0
			4362	2766	756	827	13			

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	51	Total	I	0	0
			51	51		

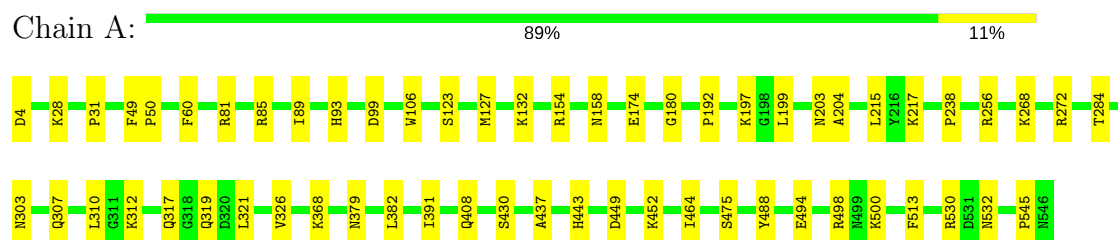
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	759	Total	O	0	0
			759	759		

### 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. 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. 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: PECTATE LYASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.49Å 95.64Å 126.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.59 – 1.50 19.31 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.59-1.50) 97.4 (19.31-1.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.222 , 0.243 0.382 , 0.385	Depositor DCC
$R_{free}$ test set	5574 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	5172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IOD

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	0.49	0/4477	0.59	0/6061

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

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	4362	0	4224	56	0
2	A	51	0	0	60	0
3	A	759	0	0	31	0
All	All	5172	0	4224	86	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 10.

All (86) 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)
2:A:1555:IOD:I	3:A:2357:HOH:O	2.21	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1576:IOD:I	3:A:2726:HOH:O	2.28	1.19
2:A:1565:IOD:I	2:A:1591:IOD:I	3.06	1.13
2:A:1588:IOD:I	3:A:2713:HOH:O	2.40	1.06
1:A:199:LEU:HB2	2:A:1555:IOD:I	2.33	0.99
1:A:199:LEU:N	2:A:1555:IOD:I	2.67	0.97
2:A:1549:IOD:I	2:A:1552:IOD:I	3.23	0.97
2:A:1552:IOD:I	3:A:2726:HOH:O	2.52	0.96
2:A:1587:IOD:I	3:A:2537:HOH:O	2.56	0.94
2:A:1558:IOD:I	3:A:2627:HOH:O	2.56	0.92
2:A:1572:IOD:I	3:A:2323:HOH:O	2.56	0.92
2:A:1552:IOD:I	2:A:1576:IOD:I	3.27	0.92
2:A:1563:IOD:I	3:A:2486:HOH:O	2.58	0.91
1:A:312:LYS:HE2	2:A:1563:IOD:I	2.41	0.90
2:A:1572:IOD:I	3:A:2107:HOH:O	2.61	0.88
2:A:1556:IOD:I	3:A:2652:HOH:O	2.61	0.88
1:A:81[B]:ARG:NH2	2:A:1569:IOD:I	2.75	0.88
2:A:1560:IOD:I	3:A:2041:HOH:O	2.61	0.87
2:A:1554:IOD:I	3:A:2290:HOH:O	2.62	0.86
1:A:317:GLN:HA	2:A:1568:IOD:I	2.46	0.85
2:A:1560:IOD:I	3:A:2333:HOH:O	2.62	0.85
1:A:49:PHE:HB3	1:A:50:PRO:HD2	1.59	0.84
2:A:1593:IOD:I	3:A:2556:HOH:O	2.65	0.84
1:A:197:LYS:HB2	1:A:256:ARG:HH22	1.45	0.81
2:A:1592:IOD:I	3:A:2494:HOH:O	2.68	0.81
2:A:1557:IOD:I	3:A:2519:HOH:O	2.69	0.80
1:A:199:LEU:CB	2:A:1555:IOD:I	3.01	0.79
2:A:1554:IOD:I	3:A:2315:HOH:O	2.72	0.78
2:A:1570:IOD:I	3:A:2247:HOH:O	2.74	0.75
2:A:1567:IOD:I	3:A:2742:HOH:O	2.73	0.75
1:A:4:ASP:N	2:A:1561:IOD:I	2.91	0.74
1:A:326:VAL:HG21	1:A:391:ILE:HD11	1.71	0.72
1:A:530:ARG:HD3	2:A:1567:IOD:I	2.60	0.72
1:A:174:GLU:OE2	2:A:1564:IOD:I	2.78	0.71
1:A:284:THR:HG21	3:A:2205:HOH:O	1.91	0.71
1:A:530:ARG:CD	2:A:1567:IOD:I	3.09	0.70
2:A:1560:IOD:I	3:A:2133:HOH:O	2.78	0.70
2:A:1574:IOD:I	3:A:2640:HOH:O	2.78	0.70
2:A:1564:IOD:I	3:A:2221:HOH:O	2.79	0.69
1:A:317:GLN:C	2:A:1568:IOD:I	3.02	0.68
1:A:379:ASN:HD21	1:A:408:GLN:HG3	1.61	0.65
1:A:215:LEU:HD21	2:A:1589:IOD:I	2.68	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLN:CA	2:A:1568:IOD:I	3.17	0.62
1:A:530:ARG:NH1	2:A:1567:IOD:I	2.95	0.61
2:A:1589:IOD:I	3:A:2092:HOH:O	2.86	0.61
1:A:530:ARG:HD2	2:A:1567:IOD:I	2.70	0.61
2:A:1592:IOD:I	3:A:2242:HOH:O	2.87	0.60
1:A:449:ASP:HA	1:A:452:LYS:HE3	1.85	0.58
1:A:500:LYS:HE3	2:A:1588:IOD:I	2.74	0.58
1:A:268:LYS:HB3	2:A:1580:IOD:I	2.74	0.58
1:A:430:SER:OG	1:A:464:ILE:HD11	2.04	0.58
1:A:192:PRO:HB3	1:A:238:PRO:HB3	1.86	0.57
1:A:49:PHE:CB	1:A:50:PRO:HD2	2.32	0.56
1:A:132:LYS:HG3	1:A:203:ASN:HB2	1.88	0.56
1:A:545:PRO:HA	2:A:1548:IOD:I	2.76	0.56
1:A:443:HIS:HD2	2:A:1547:IOD:I	2.58	0.55
1:A:123:SER:HA	3:A:2726:HOH:O	2.07	0.54
1:A:31:PRO:HG3	2:A:1573:IOD:I	2.78	0.54
1:A:89:ILE:O	1:A:93:HIS:HD2	1.91	0.54
2:A:1569:IOD:I	3:A:2136:HOH:O	2.89	0.53
1:A:530:ARG:HD2	2:A:1572:IOD:I	2.78	0.53
1:A:494:GLU:OE2	1:A:498:ARG:NE	2.41	0.53
2:A:1573:IOD:I	3:A:2018:HOH:O	2.89	0.52
1:A:199:LEU:CA	2:A:1555:IOD:I	3.26	0.52
1:A:197:LYS:HG3	1:A:256:ARG:HH12	1.75	0.52
1:A:379:ASN:ND2	1:A:408:GLN:HG3	2.25	0.52
1:A:310:LEU:HD23	1:A:321:LEU:HD21	1.93	0.50
1:A:154:ARG:HD3	2:A:1589:IOD:I	2.83	0.49
1:A:158:ASN:ND2	1:A:180:GLY:H	2.12	0.48
1:A:60:PHE:HB2	1:A:93:HIS:CE1	2.48	0.48
1:A:532:ASN:CG	2:A:1567:IOD:I	3.22	0.48
1:A:532:ASN:OD1	2:A:1567:IOD:I	3.02	0.47
1:A:49:PHE:HB3	1:A:50:PRO:CD	2.38	0.47
1:A:382:LEU:HG	1:A:437:ALA:HB1	1.96	0.46
1:A:85:ARG:NH1	2:A:1569:IOD:I	3.14	0.46
1:A:217:LYS:HB2	1:A:217:LYS:HE2	1.81	0.46
1:A:204:ALA:HB2	3:A:2228:HOH:O	2.16	0.45
1:A:317:GLN:O	2:A:1568:IOD:I	3.05	0.45
2:A:1551:IOD:I	3:A:2599:HOH:O	2.92	0.45
1:A:303:ASN:HD21	1:A:307:GLN:NE2	2.15	0.44
1:A:132:LYS:HE3	1:A:513:PHE:CE2	2.54	0.43
1:A:368:LYS:NZ	2:A:1553:IOD:I	3.18	0.42
1:A:123:SER:OG	2:A:1549:IOD:I	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LYS:CB	1:A:256:ARG:HH22	2.23	0.42
1:A:319:GLN:NE2	3:A:2497:HOH:O	2.53	0.40
1:A:443:HIS:CD2	2:A:1547:IOD:I	3.42	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	546/543 (101%)	537 (98%)	9 (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	454/449 (101%)	446 (98%)	8 (2%)	62	32

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	99	ASP
1	A	106	TRP

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Mol	Chain	Res	Type
1	A	127[A]	MET
1	A	127[B]	MET
1	A	272	ARG
1	A	475	SER
1	A	488	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	75	GLN
1	A	93	HIS
1	A	158	ASN
1	A	307	GLN
1	A	379	ASN
1	A	443	HIS
1	A	499	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 51 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 [i](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.