



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 12:00 PM EDT

PDB ID : 3EI1 / pdb_00003eii
Title : Zinc-bound glycoside hydrolase 61 E from Thielavia terrestris
Authors : Salbo, R.; Welner, D.; Lo Leggio, L.; Harris, P.; McFarland, K.
Deposited on : 2008-09-16
Resolution : 2.25 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

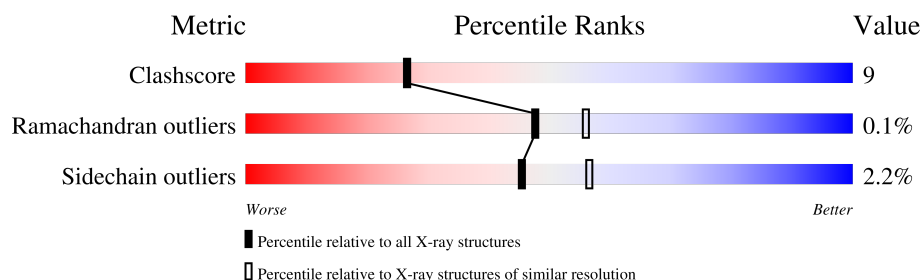
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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
5	GOL	C	2647	-	-	X	-

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	220.92Å 220.92Å 220.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25	Depositor
% Data completeness (in resolution range)	93.2 (20.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.251	Depositor
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.000	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.045 for k,h,-l	Xtriage
Total number of atoms	7221	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5412e-03.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

3 Model quality

3.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, SO4, ZN

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	0.63	1/1659 (0.1%)	0.97	3/2284 (0.1%)
1	B	0.60	0/1659	0.97	4/2284 (0.2%)
1	C	0.63	0/1659	0.98	3/2284 (0.1%)
1	D	0.60	0/1659	0.97	5/2284 (0.2%)
All	All	0.61	1/6636 (0.0%)	0.97	15/9136 (0.2%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	SER	C-O	-5.67	1.17	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	PRO	N-CA-C	7.45	123.17	113.86
1	B	5	PRO	N-CA-C	6.81	122.38	113.86
1	D	5	PRO	N-CA-C	6.79	122.35	113.86
1	A	5	PRO	N-CA-C	5.99	122.51	114.18
1	C	4	TRP	CA-C-N	5.81	125.43	119.56
1	C	4	TRP	C-N-CA	5.81	125.43	119.56
1	B	4	TRP	N-CA-C	-5.50	99.25	108.94
1	D	10	GLY	N-CA-C	5.45	118.32	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	ILE	N-CA-C	5.38	116.45	108.65
1	D	133	LEU	N-CA-C	-5.33	101.01	109.59
1	B	6	ARG	N-CA-C	5.30	117.12	109.07
1	D	4	TRP	CA-C-N	5.26	124.87	119.56
1	D	4	TRP	C-N-CA	5.26	124.87	119.56
1	B	133	LEU	N-CA-C	-5.16	100.77	109.07
1	A	8	ASN	CB-CA-C	-5.10	110.67	116.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	64	PRO	Mainchain

3.2 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	1599	0	1487	22	1
1	B	1599	0	1487	35	0
1	C	1599	0	1487	26	1
1	D	1599	0	1487	34	1
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	14	0	13	0	0
3	B	14	0	13	1	0
3	C	14	0	13	0	1
3	D	14	0	13	4	0
4	A	15	0	0	0	0
4	B	20	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	C	6	0	8	6	0
5	D	6	0	8	1	0
6	A	183	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	151	0	0	5	0
6	C	192	0	0	5	3
6	D	170	0	0	10	2
All	All	7221	0	6016	117	5

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 9.

All (117) 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:D:51:ASN:HD22	3:D:601:NAG:H82	1.34	0.93
1:C:135:ARG:HG2	6:C:4615:HOH:O	1.69	0.90
1:C:107:ALA:O	1:C:194:VAL:HG21	1.89	0.72
1:D:35:GLN:HG3	6:D:4228:HOH:O	1.90	0.72
1:B:34:PRO:HD2	6:B:4250:HOH:O	1.92	0.70
1:B:107:ALA:O	1:B:194:VAL:HG21	1.92	0.70
1:D:51:ASN:HD22	3:D:601:NAG:C8	2.05	0.69
1:D:51:ASN:ND2	3:D:601:NAG:C8	2.57	0.68
1:D:51:ASN:ND2	3:D:601:NAG:H82	2.07	0.68
1:B:14:GLN:HG2	1:B:15:GLN:NE2	2.11	0.65
1:A:171:ASN:O	6:A:4341:HOH:O	2.15	0.64
1:D:112:PRO:HG3	6:D:4509:HOH:O	1.98	0.63
1:C:104:THR:OG1	1:C:110:THR:OG1	2.17	0.61
1:C:151:GLN:HE22	5:C:2647:GOL:H31	1.66	0.61
1:B:85:ILE:HD12	1:B:131:TYR:HB3	1.82	0.61
1:A:18:LYS:HE2	1:A:22:TRP:CE2	2.36	0.61
1:A:154:ILE:HG22	1:A:155:SER:N	2.16	0.61
1:B:116:LYS:HD3	6:B:4454:HOH:O	2.01	0.60
1:A:171:ASN:HB2	6:A:4321:HOH:O	2.02	0.60
1:C:199:GLN:HG2	6:D:4486:HOH:O	2.02	0.59
1:B:171:ASN:HB3	6:B:4410:HOH:O	2.02	0.58
1:D:70:GLY:HA3	1:D:139:ILE:O	2.03	0.58
1:A:107:ALA:O	1:A:194:VAL:HG21	2.03	0.58
1:B:70:GLY:HA3	1:B:139:ILE:O	2.03	0.58
1:A:43:PRO:HG3	6:A:4677:HOH:O	2.04	0.57
1:C:70:GLY:HA3	1:C:139:ILE:O	2.03	0.57
1:D:104:THR:OG1	1:D:110:THR:HB	2.05	0.57
1:D:14:GLN:NE2	1:D:15:GLN:HE22	2.02	0.56
1:B:47:PRO:HG3	6:B:4585:HOH:O	2.04	0.56
1:C:167:THR:HG23	6:C:4577:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLY:HA3	1:A:139:ILE:O	2.05	0.56
1:A:79:VAL:HG22	1:A:88:TRP:CE3	2.40	0.56
1:B:108:GLN:HG2	6:B:4150:HOH:O	2.06	0.55
1:B:51:ASN:HD22	3:B:601:NAG:H82	1.72	0.55
1:C:94:VAL:C	1:C:172:LYS:HG2	2.33	0.53
1:C:142:HIS:NE2	5:C:2647:GOL:H11	2.22	0.53
1:B:100:GLU:HG2	1:B:205:VAL:CG2	2.39	0.53
1:C:151:GLN:HE22	5:C:2647:GOL:C3	2.20	0.53
1:D:100:GLU:HG2	1:D:205:VAL:CG2	2.39	0.53
1:A:1:HIS:CE1	6:A:4281:HOH:O	2.61	0.53
1:D:154:ILE:HG22	1:D:155:SER:N	2.24	0.53
1:C:199:GLN:HB3	6:C:4685:HOH:O	2.08	0.53
1:D:105:PHE:HB3	6:D:4199:HOH:O	2.09	0.52
1:C:154:ILE:CG2	1:C:155:SER:N	2.72	0.52
1:D:100:GLU:HG2	1:D:205:VAL:HG21	1.92	0.52
1:C:151:GLN:HE22	5:C:2647:GOL:H12	1.75	0.51
1:B:152:PHE:HB3	1:B:154:ILE:HD11	1.93	0.51
1:D:14:GLN:NE2	1:D:15:GLN:NE2	2.59	0.51
1:D:31:VAL:HG22	6:D:4039:HOH:O	2.11	0.51
1:D:45:PRO:HB3	1:D:86:ASN:O	2.11	0.51
1:C:142:HIS:NE2	5:C:2647:GOL:C1	2.73	0.51
1:B:99:TYR:C	1:B:99:TYR:CD1	2.88	0.50
1:A:3:THR:HG23	1:A:25:ASN:OD1	2.12	0.50
1:D:154:ILE:CG2	1:D:155:SER:N	2.75	0.49
1:A:104:THR:HB	1:A:110:THR:OG1	2.11	0.49
1:A:73:GLN:OE1	1:A:200:ASN:HB3	2.13	0.49
1:A:45:PRO:HB3	1:A:86:ASN:O	2.13	0.49
1:B:128:LYS:HB2	1:B:128:LYS:NZ	2.28	0.49
1:D:112:PRO:CG	6:D:4509:HOH:O	2.58	0.49
1:B:100:GLU:OE2	1:B:102:HIS:HE1	1.96	0.48
1:B:22:TRP:CZ2	1:B:23:GLN:NE2	2.81	0.48
1:B:154:ILE:CG2	1:B:155:SER:N	2.77	0.48
1:C:6:ARG:HG2	1:C:11:ALA:C	2.38	0.48
1:D:155:SER:HA	6:D:4143:HOH:O	2.14	0.48
1:A:22:TRP:CD2	1:A:23:GLN:HG3	2.48	0.48
1:B:73:GLN:OE1	1:B:200:ASN:HB3	2.14	0.48
1:D:23:GLN:HB2	6:D:4477:HOH:O	2.14	0.47
1:B:45:PRO:HB3	1:B:86:ASN:O	2.14	0.47
1:B:78:ARG:HB2	1:B:132:TYR:CE2	2.49	0.47
1:B:100:GLU:HG2	1:B:205:VAL:HG21	1.97	0.47
1:A:23:GLN:HB2	6:A:4010:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:PRO:O	1:B:116:LYS:HD2	2.16	0.46
1:A:158:GLN:C	1:A:159:LEU:HD12	2.41	0.46
1:C:14:GLN:HG2	1:C:15:GLN:NE2	2.30	0.46
1:B:153:TYR:C	1:B:154:ILE:HG13	2.42	0.45
1:C:154:ILE:HG22	1:C:155:SER:N	2.30	0.45
1:D:18:LYS:HD2	6:D:4654:HOH:O	2.17	0.45
1:A:154:ILE:CG2	1:A:155:SER:N	2.79	0.45
1:D:152:PHE:HB3	1:D:154:ILE:HD11	1.99	0.45
1:A:22:TRP:CE2	1:A:23:GLN:HG3	2.52	0.45
1:B:154:ILE:HG22	1:B:155:SER:N	2.30	0.45
1:D:153:TYR:C	1:D:154:ILE:HG13	2.40	0.45
1:D:85:ILE:O	1:D:85:ILE:HG13	2.15	0.45
1:C:45:PRO:HB3	1:C:86:ASN:O	2.17	0.44
1:B:128:LYS:NZ	1:B:128:LYS:CB	2.81	0.44
1:C:109:LEU:HB2	6:C:4125:HOH:O	2.17	0.44
1:D:68:HIS:HE1	5:D:2647:GOL:O2	2.00	0.44
1:B:169:PRO:O	1:B:172:LYS:HD3	2.18	0.43
1:C:151:GLN:NE2	5:C:2647:GOL:H31	2.32	0.43
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.88	0.43
1:A:3:THR:OG1	1:A:5:PRO:HD3	2.17	0.43
1:B:152:PHE:HB3	1:B:154:ILE:CD1	2.49	0.43
1:D:18:LYS:HB2	6:D:4530:HOH:O	2.18	0.43
1:D:97:LYS:HD3	1:D:100:GLU:HB3	2.01	0.43
1:D:78:ARG:HG3	1:D:132:TYR:CZ	2.53	0.43
1:D:63:ASN:HA	1:D:64:PRO:C	2.43	0.43
1:A:85:ILE:HD12	1:A:131:TYR:HB3	2.01	0.43
1:D:14:GLN:CD	1:D:15:GLN:HE22	2.26	0.42
1:C:27:TYR:HB3	1:C:153:TYR:CE1	2.55	0.42
1:B:99:TYR:CD1	1:B:100:GLU:N	2.88	0.42
1:B:13:TRP:CE3	1:B:18:LYS:HA	2.54	0.42
1:C:3:THR:OG1	1:C:5:PRO:HD3	2.20	0.42
1:B:27:TYR:HB3	1:B:153:TYR:CE1	2.55	0.42
1:B:73:GLN:HB2	1:B:137:GLU:OE1	2.19	0.41
1:B:123:ILE:O	1:B:124:PRO:C	2.63	0.41
1:D:192:TYR:HA	1:D:193:PRO:C	2.45	0.41
1:B:3:THR:C	1:B:5:PRO:HD3	2.45	0.41
1:A:128:LYS:HB2	1:A:128:LYS:NZ	2.36	0.41
1:D:73:GLN:OE1	1:D:200:ASN:HB3	2.20	0.41
1:C:123:ILE:O	1:C:124:PRO:C	2.63	0.41
1:D:13:TRP:CG	1:D:18:LYS:HG3	2.55	0.41
1:A:27:TYR:HB3	1:A:153:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:VAL:HG22	1:B:88:TRP:CE3	2.56	0.41
1:C:73:GLN:OE1	1:C:200:ASN:HB3	2.20	0.41
1:D:27:TYR:HB3	1:D:153:TYR:CE1	2.56	0.41
1:C:167:THR:CG2	6:C:4577:HOH:O	2.65	0.40
1:C:18:LYS:HB2	1:C:18:LYS:NZ	2.37	0.40

All (5) 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:D:191:TYR:O	6:C:4120:HOH:O[12_665]	1.95	0.25
3:C:601:NAG:O4	6:C:4202:HOH:O[16_556]	2.09	0.11
1:C:172:LYS:O	6:D:4223:HOH:O[6_566]	2.10	0.10
1:A:182:THR:OG1	6:C:4323:HOH:O[45_545]	2.16	0.04
6:D:4287:HOH:O	6:D:4495:HOH:O[12_665]	2.19	0.01

3.3 Torsion angles

3.3.1 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	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
1	B	206/208 (99%)	200 (97%)	6 (3%)	0	100	100
1	C	206/208 (99%)	200 (97%)	6 (3%)	0	100	100
1	D	206/208 (99%)	200 (97%)	5 (2%)	1 (0%)	24	24
All	All	824/832 (99%)	798 (97%)	25 (3%)	1 (0%)	48	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	64	PRO

3.3.2 Protein sidechains ⓘ

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	170/170 (100%)	166 (98%)	4 (2%)	43	54
1	B	170/170 (100%)	166 (98%)	4 (2%)	43	54
1	C	170/170 (100%)	167 (98%)	3 (2%)	51	63
1	D	170/170 (100%)	166 (98%)	4 (2%)	43	54
All	All	680/680 (100%)	665 (98%)	15 (2%)	45	56

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TYR
1	A	5	PRO
1	A	18	LYS
1	A	108	GLN
1	B	2	TYR
1	B	128	LYS
1	B	133	LEU
1	B	172	LYS
1	C	2	TYR
1	C	100	GLU
1	C	172	LYS
1	D	2	TYR
1	D	84	ASP
1	D	85	ILE
1	D	128	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	63	ASN
1	A	108	GLN
1	A	199	GLN

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Mol	Chain	Res	Type
1	B	14	GLN
1	B	63	ASN
1	B	200	ASN
1	C	35	GLN
1	C	151	GLN
1	C	171	ASN
1	D	14	GLN
1	D	63	ASN
1	D	171	ASN

3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 23 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - 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.

3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

4 Fit of model and data

4.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

4.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

4.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

4.4 Ligands

EDS failed to run properly - this section is therefore empty.

4.5 Other polymers

EDS failed to run properly - this section is therefore empty.