



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2016 – 02:09 PM EST

PDB ID : 1DYS
Title : Endoglucanase CEL6B from Humicola insolens
Authors : Davies, G.J.; Brzozowski, A.M.; Dauter, M.; Varrot, A.; Schulein, M.
Deposited on : 2000-02-08
Resolution : 1.60 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

<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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

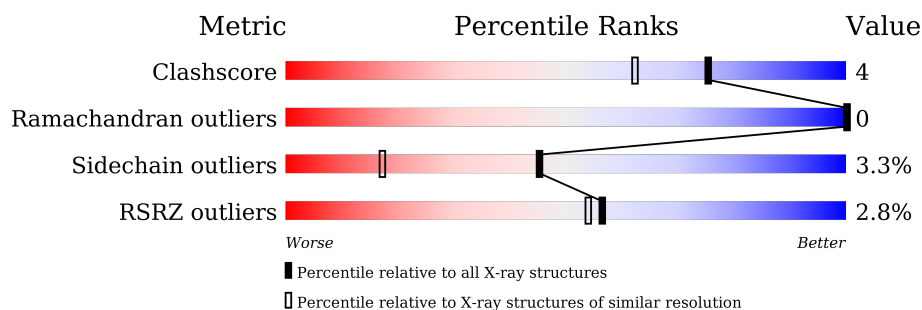
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	348	<div> <div>4%</div> <div>82%</div> <div>15%</div> <div>...</div> </div>
1	B	348	<div> <div>2%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6181 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 ENDOGLUCANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	6	0
			2641	1644	470	518	9			
1	B	345	Total	C	N	O	S	0	4	0
			2639	1644	470	516	9			

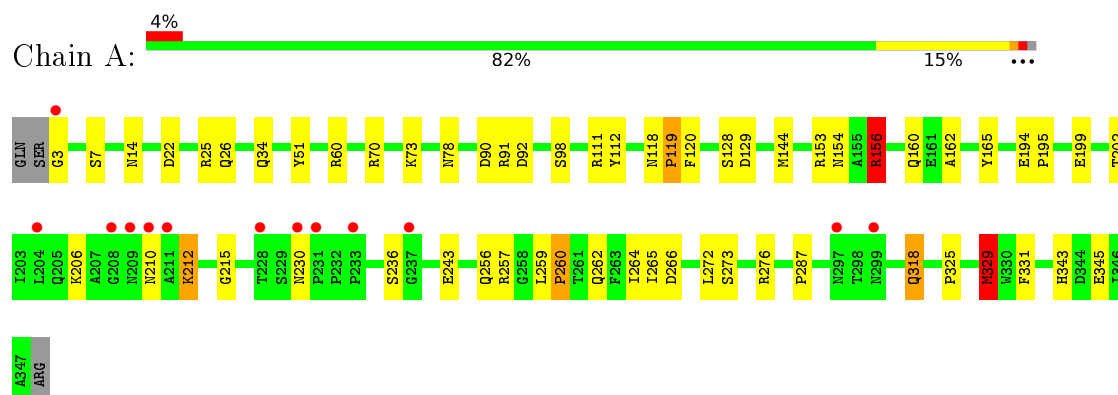
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	456	Total	O	0	0
			456	456		
2	B	445	Total	O	0	0
			445	445		

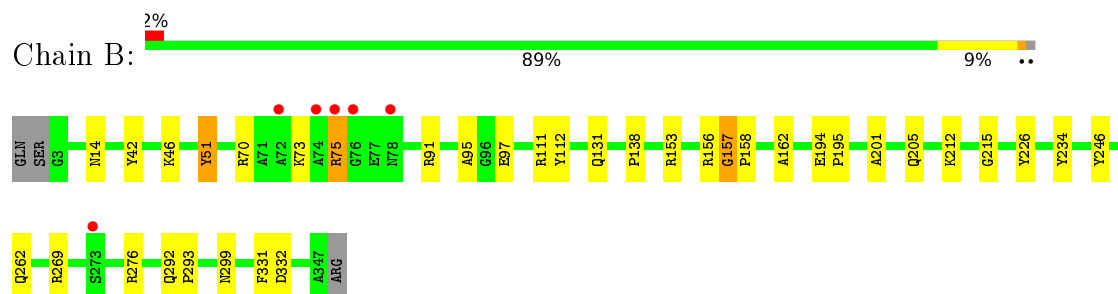
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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



• Molecule 1: ENDOGLUCANASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.92Å 104.45Å 53.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.60 14.98 – 1.62	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-1.60) 97.5 (14.98-1.62)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 1.62Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.240 0.187 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.045 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6181	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.58	0/2731	1.38	25/3714 (0.7%)
1	B	0.63	0/2719	1.37	17/3698 (0.5%)
All	All	0.61	0/5450	1.38	42/7412 (0.6%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ARG	NE-CZ-NH2	-13.35	113.63	120.30
1	A	60	ARG	CD-NE-CZ	11.74	140.04	123.60
1	A	91	ARG	NE-CZ-NH1	11.39	126.00	120.30
1	B	70	ARG	NE-CZ-NH1	9.69	125.15	120.30
1	A	25	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	B	111	ARG	NE-CZ-NH2	-9.43	115.59	120.30
1	A	91	ARG	NE-CZ-NH2	-9.15	115.73	120.30
1	B	111	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	A	153	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	B	276	ARG	NE-CZ-NH1	-8.15	116.22	120.30
1	B	70	ARG	CD-NE-CZ	8.09	134.93	123.60
1	A	60	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	A	156	ARG	CD-NE-CZ	7.60	134.24	123.60
1	A	165	TYR	CB-CG-CD2	7.44	125.46	121.00
1	A	60	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	B	51	TYR	CB-CG-CD1	-7.06	116.76	121.00
1	B	331	PHE	CB-CG-CD2	-6.76	116.07	120.80
1	B	332	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	A	257	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	B	331	PHE	CB-CG-CD1	6.47	125.33	120.80
1	A	120	PHE	CB-CG-CD2	-6.36	116.35	120.80
1	A	119	PRO	N-CA-CB	6.23	110.77	103.30
1	A	111	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	269	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	A	266	ASP	CB-CG-OD1	6.00	123.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	A	156	ARG	CG-CD-NE	5.84	124.06	111.80
1	B	91	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	91	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	264	ILE	N-CA-CB	5.67	123.84	110.80
1	B	226	TYR	CB-CG-CD2	5.66	124.40	121.00
1	A	92	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	329	MET	CA-CB-CG	5.39	122.47	113.30
1	A	70	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	318	GLN	OE1-CD-NE2	5.34	134.18	121.90
1	B	131	GLN	O-C-N	5.32	131.21	122.70
1	A	260	PRO	N-CA-CB	5.21	109.55	103.30
1	B	138	PRO	C-N-CA	5.20	134.69	121.70
1	A	129	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	111	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	276	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	157	GLY	CA-C-O	5.05	129.69	120.60

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	2641	0	2534	24	0
1	B	2639	0	2532	16	0
2	A	456	0	0	6	0
2	B	445	0	0	5	0
All	All	6181	0	5066	40	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 4.

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:156:ARG:HG3	1:A:156:ARG:HH11	1.59	0.68
1:B:299:ASN:HB3	2:B:2400:HOH:O	1.96	0.65
1:B:201:ALA:O	1:B:205:GLN:HG3	1.98	0.64
1:A:272:LEU:HD12	1:A:287:PRO:HB2	1.83	0.61
1:B:75:ARG:HD2	2:B:2143:HOH:O	2.02	0.60
1:A:343:HIS:CE1	1:A:345:GLU:HG3	2.37	0.60
1:A:259:LEU:HB3	1:A:260:PRO:HD2	1.85	0.57
1:A:318:GLN:NE2	2:A:2423:HOH:O	2.39	0.55
1:B:95:ALA:HB3	2:B:2171:HOH:O	2.08	0.52
1:A:243:GLU:HB3	1:A:265:ILE:HD13	1.91	0.51
1:B:153:ARG:HD2	2:B:2251:HOH:O	2.11	0.51
1:A:3:GLY:N	2:A:2001:HOH:O	2.43	0.51
1:A:144:MET:HG2	1:A:156:ARG:NH1	2.27	0.49
1:A:90:ASP:HA	1:A:98:SER:HB2	1.95	0.49
1:B:14:ASN:HA	1:B:51:TYR:CZ	2.47	0.49
1:A:212:LYS:HD3	2:A:2304:HOH:O	2.13	0.48
1:A:26:GLN:NE2	2:A:2065:HOH:O	2.46	0.48
1:B:194:GLU:HB2	1:B:195:PRO:HD3	1.96	0.47
1:A:325:PRO:HB2	1:A:329:MET:HB3	1.97	0.46
1:B:215:GLY:HA3	1:B:262:GLN:O	2.16	0.45
1:B:97:GLU:HG2	2:B:2181:HOH:O	2.16	0.45
1:A:118:ASN:HB2	1:A:119:PRO:HD3	2.00	0.44
1:B:194:GLU:N	1:B:195:PRO:CD	2.81	0.44
1:A:14:ASN:HA	1:A:51:TYR:CZ	2.53	0.43
1:A:202:THR:HG22	1:A:206:LYS:HE2	2.01	0.43
1:A:144:MET:HG2	1:A:156:ARG:HH11	1.83	0.43
1:A:154:ASN:ND2	2:A:2290:HOH:O	2.52	0.43
1:A:215:GLY:HA3	1:A:262:GLN:O	2.19	0.42
1:B:112:TYR:CE2	1:B:162:ALA:HB1	2.54	0.42
1:B:42:TYR:CE1	1:B:46:LYS:HD3	2.55	0.42
1:B:156:ARG:HD3	1:B:156:ARG:HH11	1.63	0.42
1:B:157:GLY:N	1:B:158:PRO:CD	2.83	0.42
1:A:202:THR:O	1:A:206:LYS:HG3	2.20	0.41
1:A:194:GLU:N	1:A:195:PRO:CD	2.84	0.41
1:B:153:ARG:HH11	1:B:153:ARG:HD2	1.72	0.41
1:A:256:GLN:NE2	2:A:2377:HOH:O	2.47	0.41
1:A:112:TYR:CE2	1:A:162:ALA:HB1	2.56	0.40
1:B:292:GLN:HA	1:B:293:PRO:HD3	1.93	0.40
1:A:160:GLN:NE2	1:A:199:GLU:OE2	2.49	0.40
1:A:343:HIS:ND1	1:A:345:GLU:HG3	2.36	0.40

There are no symmetry-related clashes.

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	349/348 (100%)	336 (96%)	13 (4%)	0	100	100
1	B	347/348 (100%)	332 (96%)	15 (4%)	0	100	100
All	All	696/696 (100%)	668 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 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	281/278 (101%)	266 (95%)	15 (5%)	28	7
1	B	279/278 (100%)	275 (99%)	4 (1%)	74	53
All	All	560/556 (101%)	541 (97%)	19 (3%)	45	16

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	22	ASP
1	A	34	GLN
1	A	73	LYS
1	A	78	ASN
1	A	128[A]	SER
1	A	128[B]	SER
1	A	156	ARG

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Mol	Chain	Res	Type
1	A	210	ASN
1	A	212	LYS
1	A	230	ASN
1	A	236	SER
1	A	273	SER
1	A	329	MET
1	A	331	PHE
1	B	73	LYS
1	B	75	ARG
1	B	212	LYS
1	B	234	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	26	GLN
1	A	78	ASN
1	A	107	ASN
1	A	110	ASN
1	A	209	ASN
1	A	256	GLN
1	A	299	ASN
1	A	302	ASN
1	A	318	GLN
1	A	340	GLN
1	B	68	ASN
1	B	78	ASN
1	B	107	ASN
1	B	110	ASN
1	B	154	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

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, 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	345/348 (99%)	-0.04	13 (3%) 44 41	12, 20, 34, 48	0
1	B	345/348 (99%)	-0.10	6 (1%) 73 71	12, 20, 33, 48	0
All	All	690/696 (99%)	-0.07	19 (2%) 56 54	12, 20, 33, 48	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	ASN	4.6
1	B	74	ALA	4.2
1	B	75	ARG	3.4
1	A	3	GLY	3.3
1	A	210	ASN	2.9
1	B	72	ALA	2.7
1	B	273	SER	2.5
1	A	208	GLY	2.5
1	A	299	ASN	2.5
1	A	230	ASN	2.4
1	A	211	ALA	2.3
1	A	237	GLY	2.3
1	A	231	PRO	2.3
1	A	228	THR	2.2
1	B	76	GLY	2.2
1	B	78	ASN	2.1
1	A	233	PRO	2.1
1	A	204	LEU	2.0
1	A	297	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.