



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:01 pm BST

PDB ID : 1CBG
Title : THE CRYSTAL STRUCTURE OF A CYANOGENIC BETA-GLUCOSIDASE FROM WHITE CLOVER (TRIFOLIUM REPENS L.), A FAMILY 1 GLYCOSYL-HYDROLASE
Authors : Barrett, T.E.; Suresh, C.G.; Tolley, S.P.; Hughes, M.A.
Deposited on : 1995-07-31
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

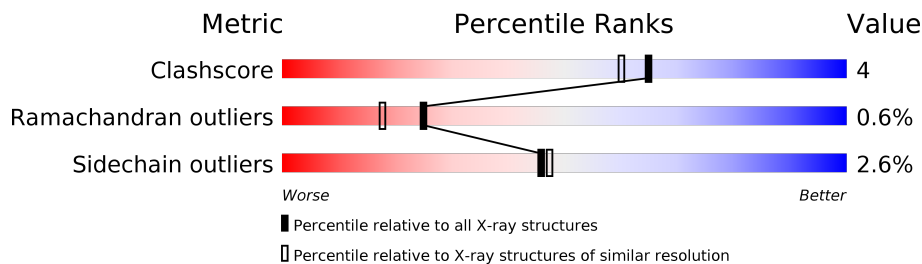
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	490	 82% 15% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4429 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 CYANOGENIC BETA-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	490	3993	2584	675	720	14	40	0	0

- Molecule 2 is water.

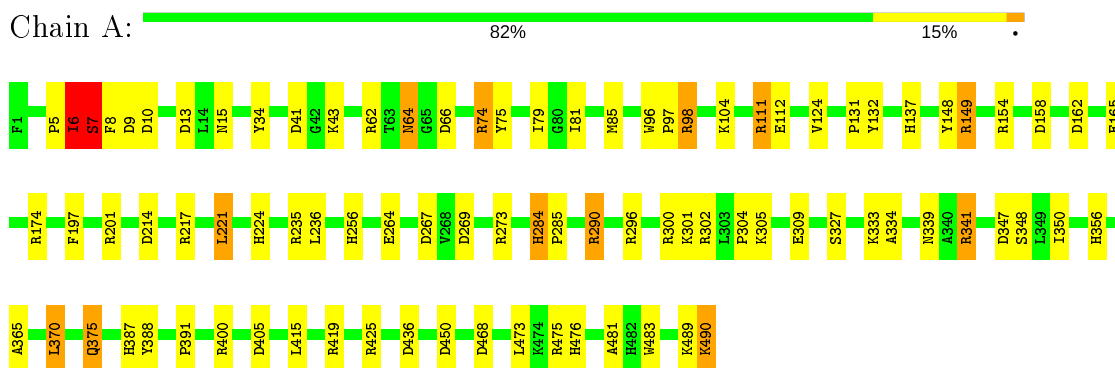
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	436	Total	O	0	0
			436	436		

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.

Note EDS was not executed.

- Molecule 1: CYANOGENIC BETA-GLUCOSIDASE



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	70.33Å 70.33Å 249.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.00 – 2.15	Depositor
% Data completeness (in resolution range)	95.0 (9.00-2.15)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR 3.1	Depositor
R, R_{free}	0.195 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4429	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

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	0.89	7/4119 (0.2%)	1.68	66/5585 (1.2%)

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	A	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	ILE	C-N	-21.93	0.83	1.34
1	A	7	SER	C-N	-12.75	1.04	1.34
1	A	111	ARG	C-N	-10.60	1.09	1.34
1	A	334	ALA	C-N	-8.44	1.18	1.34
1	A	301	LYS	CA-CB	-6.12	1.40	1.53
1	A	104	LYS	CD-CE	5.99	1.66	1.51
1	A	300	ARG	CD-NE	-5.62	1.36	1.46

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ARG	CD-NE-CZ	32.03	168.44	123.60
1	A	62	ARG	CD-NE-CZ	23.49	156.49	123.60
1	A	6	ILE	O-C-N	-22.96	85.96	122.70
1	A	74	ARG	NE-CZ-NH2	-19.34	110.63	120.30
1	A	74	ARG	NE-CZ-NH1	17.78	129.19	120.30
1	A	74	ARG	CD-NE-CZ	13.46	142.45	123.60
1	A	400	ARG	NE-CZ-NH1	11.23	125.92	120.30
1	A	217	ARG	NE-CZ-NH1	10.61	125.60	120.30
1	A	341	ARG	NE-CZ-NH2	-10.10	115.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ARG	NE-CZ-NH2	-9.55	115.52	120.30
1	A	468	ASP	CB-CG-OD1	9.46	126.81	118.30
1	A	235	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	A	290	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	405	ASP	CB-CG-OD2	-8.86	110.32	118.30
1	A	10	ASP	CB-CG-OD1	8.70	126.13	118.30
1	A	111	ARG	C-N-CA	8.57	143.12	121.70
1	A	302	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	419	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	A	111	ARG	CB-CA-C	8.14	126.69	110.40
1	A	13	ASP	CB-CG-OD1	7.70	125.23	118.30
1	A	300	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	A	296	ARG	NE-CZ-NH2	7.65	124.13	120.30
1	A	269	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	405	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	98	ARG	NE-CZ-NH2	7.45	124.03	120.30
1	A	111	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	A	149	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	269	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	A	475	ARG	CD-NE-CZ	6.52	132.73	123.60
1	A	111	ARG	O-C-N	-6.45	112.37	122.70
1	A	221	LEU	CA-CB-CG	6.42	130.06	115.30
1	A	300	ARG	CD-NE-CZ	6.40	132.56	123.60
1	A	347	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	41	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	111	ARG	CB-CG-CD	6.18	127.67	111.60
1	A	201	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	34	TYR	CA-CB-CG	6.08	124.95	113.40
1	A	296	ARG	NH1-CZ-NH2	-6.05	112.75	119.40
1	A	158	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	327	SER	N-CA-CB	-6.00	101.51	110.50
1	A	154	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	149	ARG	CD-NE-CZ	5.82	131.75	123.60
1	A	490	LYS	N-CA-CB	5.79	121.01	110.60
1	A	341	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	235	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	468	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	264	GLU	CA-CB-CG	5.68	125.90	113.40
1	A	158	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	296	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	235	ARG	CD-NE-CZ	5.54	131.35	123.60
1	A	111	ARG	CA-C-N	5.33	128.93	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	450	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	267	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	162	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	415	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	425	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	214	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	300	ARG	CG-CD-NE	5.11	122.53	111.80
1	A	489	LYS	N-CA-C	5.11	124.78	111.00
1	A	154	ARG	C-N-CA	5.09	134.44	121.70
1	A	419	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	137	HIS	C-N-CA	5.08	134.41	121.70
1	A	197	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	A	450	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	436	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	PRO	Mainchain
1	A	6	ILE	Mainchain

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	3993	0	3840	32	0
2	A	436	0	0	13	0
All	All	4429	0	3840	32	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 (32) 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:387:HIS:HD2	2:A:921:HOH:O	1.28	1.15
1:A:483:TRP:HD1	2:A:900:HOH:O	0.83	1.14
1:A:483:TRP:CD1	2:A:900:HOH:O	1.64	0.96
1:A:15:ASN:ND2	2:A:904:HOH:O	2.31	0.63
1:A:305:LYS:HE3	2:A:915:HOH:O	2.01	0.61
1:A:256:HIS:HD2	2:A:635:HOH:O	1.83	0.60
1:A:132:TYR:OH	2:A:575:HOH:O	2.05	0.55
1:A:64:ASN:HD22	1:A:66:ASP:H	1.55	0.54
1:A:476:HIS:HE1	2:A:905:HOH:O	1.92	0.51
1:A:43:LYS:HG3	1:A:98:ARG:HA	1.93	0.51
1:A:388:TYR:O	1:A:391:PRO:HD3	2.12	0.50
1:A:75:TYR:O	1:A:79:ILE:HG12	2.11	0.50
1:A:387:HIS:CD2	2:A:921:HOH:O	2.19	0.49
1:A:375:GLN:HE21	1:A:375:GLN:H	1.60	0.48
1:A:348:SER:HB2	1:A:350:ILE:HD12	1.95	0.48
1:A:74:ARG:NH2	1:A:473:LEU:HB2	2.28	0.48
1:A:356:HIS:HD2	2:A:824:HOH:O	1.96	0.48
1:A:273:ARG:HB2	1:A:350:ILE:HD11	1.95	0.48
1:A:85:MET:HE2	1:A:481:ALA:HB1	1.96	0.47
1:A:165:GLU:HB2	1:A:236:LEU:HD21	1.97	0.45
1:A:284:HIS:HB3	1:A:290:ARG:O	2.16	0.45
1:A:339:ASN:CG	1:A:339:ASN:O	2.56	0.44
1:A:333:LYS:HE3	2:A:875:HOH:O	2.18	0.44
1:A:256:HIS:HE1	2:A:906:HOH:O	2.01	0.43
1:A:96:TRP:HB3	1:A:97:PRO:HD3	2.01	0.42
1:A:365:ALA:HB3	1:A:370:LEU:HG	2.01	0.42
1:A:81:ILE:HG23	1:A:85:MET:HE3	2.00	0.42
1:A:224:HIS:CD2	1:A:304:PRO:HB2	2.54	0.42
1:A:148:TYR:O	1:A:149:ARG:HB2	2.19	0.41
1:A:79:ILE:HD12	1:A:124:VAL:HG22	2.03	0.41
1:A:284:HIS:CB	1:A:285:PRO:HD3	2.51	0.40
1:A:131:PRO:HD2	2:A:599:HOH:O	2.22	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	488/490 (100%)	471 (96%)	14 (3%)	3 (1%)	25 18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	8	PHE
1	A	6	ILE

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	417/417 (100%)	406 (97%)	11 (3%)	46 47

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	64	ASN
1	A	111	ARG
1	A	112	GLU
1	A	221	LEU
1	A	284	HIS
1	A	309	GLU
1	A	341	ARG
1	A	370	LEU
1	A	375	GLN
1	A	490	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	137	HIS
1	A	224	HIS
1	A	226	GLN
1	A	230	HIS
1	A	256	HIS
1	A	284	HIS
1	A	351	ASN
1	A	375	GLN
1	A	387	HIS
1	A	476	HIS
1	A	482	HIS

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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	334:ALA	C	335:PRO	N	1.18
1	A	111:ARG	C	112:GLU	N	1.09
1	A	7:SER	C	8:PHE	N	1.04
1	A	6:ILE	C	7:SER	N	0.83

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.