



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:03 am GMT

PDB ID : 2AMG
Title : STRUCTURE OF HYDROLASE (GLYCOSIDASE)
Authors : Morishita, Y.; Hasegawa, K.; Matsuura, Y.; Kubota, M.; Sakai, S.; Katsube, Y.
Deposited on : 1996-12-23
Resolution : 2.00 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

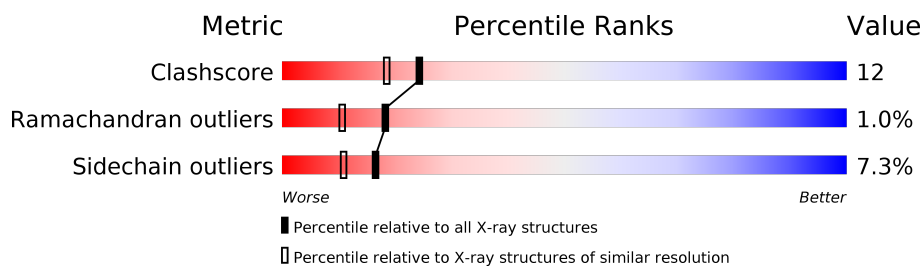
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	418	 74% 20% 5% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3459 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 1,4-ALPHA-D-GLUCAN MALTOTETRAHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3279	2061	593	615	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	ASP	SER	CONFLICT	UNP P13507

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is water.

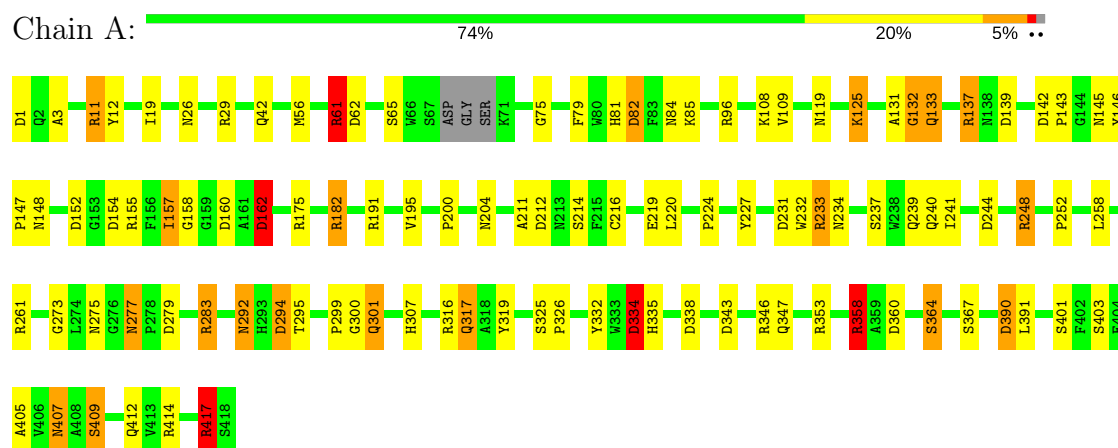
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total	O	0	0
			178	178		

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 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 ($RSRZ > 2$). 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.

Note EDS was not executed.

• Molecule 1: 1,4-ALPHA-D-GLUCAN MALTOTETRAHYDROLASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.60Å 170.50Å 46.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	91.6 (10.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT, X-PLOR	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3459	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.84	1/3383 (0.0%)	1.69	50/4604 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ASP	CA-CB	5.83	1.66	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ARG	CD-NE-CZ	38.47	177.46	123.60
1	A	175	ARG	NE-CZ-NH1	19.68	130.14	120.30
1	A	175	ARG	CD-NE-CZ	18.17	149.03	123.60
1	A	417	ARG	NE-CZ-NH1	16.15	128.38	120.30
1	A	191	ARG	NE-CZ-NH1	14.59	127.60	120.30
1	A	82	ASP	CB-CG-OD1	-13.26	106.36	118.30
1	A	11	ARG	NE-CZ-NH1	12.37	126.48	120.30
1	A	175	ARG	NE-CZ-NH2	-11.08	114.76	120.30
1	A	19	ILE	CB-CG1-CD1	9.92	141.66	113.90
1	A	358	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	A	283	ARG	CA-CB-CG	9.36	133.99	113.40
1	A	96	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	A	417	ARG	NE-CZ-NH2	-9.27	115.66	120.30
1	A	390	ASP	CB-CG-OD1	8.93	126.33	118.30
1	A	414	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	358	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	334	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	A	409	SER	N-CA-CB	7.92	122.38	110.50
1	A	182	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	A	82	ASP	CB-CG-OD2	7.31	124.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	ASP	CB-CG-OD1	7.26	124.83	118.30
1	A	11	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	191	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	248	ARG	CD-NE-CZ	7.19	133.67	123.60
1	A	82	ASP	CB-CA-C	-7.17	96.07	110.40
1	A	334	ASP	CA-CB-CG	-6.69	98.68	113.40
1	A	360	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	61	ARG	NE-CZ-NH2	6.47	123.53	120.30
1	A	139	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	231	ASP	CB-CG-OD1	6.14	123.82	118.30
1	A	283	ARG	CD-NE-CZ	6.11	132.16	123.60
1	A	3	ALA	CA-C-N	6.05	128.31	116.20
1	A	294	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	364	SER	N-CA-CB	5.92	119.39	110.50
1	A	152	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	182	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	343	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	300	GLY	C-N-CA	5.75	136.08	121.70
1	A	162	ASP	CB-CG-OD1	-5.74	113.13	118.30
1	A	137	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	353	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	294	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	338	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	360	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	346	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	19	ILE	CA-CB-CG1	5.11	120.70	111.00
1	A	82	ASP	CA-CB-CG	-5.09	102.21	113.40
1	A	417	ARG	CD-NE-CZ	5.04	130.66	123.60
1	A	148	ASN	CB-CA-C	5.02	120.44	110.40
1	A	227	TYR	CB-CG-CD2	-5.00	118.00	121.00

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	3279	0	3000	78	0
2	A	2	0	0	0	0
3	A	178	0	0	4	0
All	All	3459	0	3000	78	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 12.

All (78) 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:233:ARG:HG2	1:A:241:ILE:HG12	1.47	0.96
1:A:277:ASN:HD22	1:A:279:ASP:H	1.17	0.93
1:A:145:ASN:HD21	1:A:154:ASP:HB3	1.40	0.84
1:A:237:SER:H	1:A:240:GLN:HE21	1.23	0.84
1:A:317:GLN:H	1:A:317:GLN:HE21	1.23	0.80
1:A:182:ARG:HD2	1:A:211:ALA:HB2	1.63	0.80
1:A:61:ARG:HD3	1:A:82:ASP:HB2	1.66	0.78
1:A:11:ARG:HH12	1:A:204:ASN:HD22	1.31	0.76
1:A:277:ASN:ND2	1:A:279:ASP:H	1.87	0.73
1:A:132:GLY:O	1:A:133:GLN:HG2	1.89	0.73
1:A:409:SER:O	1:A:412:GLN:HG3	1.90	0.71
1:A:216:CYS:O	1:A:252:PRO:HD2	1.92	0.70
1:A:244:ASP:O	1:A:248:ARG:HG3	1.92	0.70
1:A:233:ARG:CG	1:A:241:ILE:HG12	2.21	0.70
1:A:358:ARG:HG3	3:A:607:HOH:O	1.90	0.69
1:A:145:ASN:ND2	1:A:155:ARG:H	1.92	0.67
1:A:277:ASN:O	1:A:283:ARG:HG3	1.94	0.67
1:A:157:ILE:HG22	1:A:158:GLY:H	1.64	0.63
1:A:292:ASN:ND2	1:A:295:THR:H	1.96	0.63
1:A:292:ASN:HD21	1:A:294:ASP:HB3	1.64	0.62
1:A:237:SER:H	1:A:240:GLN:NE2	1.94	0.61
1:A:292:ASN:HD22	1:A:292:ASN:C	2.04	0.61
1:A:157:ILE:HG22	1:A:158:GLY:N	2.16	0.61
1:A:292:ASN:ND2	1:A:294:ASP:H	1.99	0.60
1:A:61:ARG:HD2	1:A:84:ASN:HB3	1.85	0.59
1:A:232:TRP:CE2	1:A:233:ARG:HD3	2.39	0.58
1:A:219:GLU:OE1	3:A:661:HOH:O	2.17	0.57
1:A:407:ASN:C	1:A:407:ASN:HD22	2.08	0.57
1:A:258:LEU:HB2	1:A:273:GLY:HA3	1.86	0.57
1:A:317:GLN:NE2	1:A:317:GLN:H	2.00	0.57
1:A:277:ASN:HD22	1:A:279:ASP:N	1.97	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ASN:HD22	1:A:29:ARG:HE	1.53	0.56
1:A:82:ASP:HB3	1:A:84:ASN:H	1.71	0.56
1:A:145:ASN:HD21	1:A:154:ASP:CB	2.14	0.55
1:A:405:ALA:HB2	1:A:417:ARG:HG2	1.89	0.54
1:A:200:PRO:HB2	1:A:248:ARG:HB2	1.90	0.54
1:A:137:ARG:NH2	1:A:146:TYR:O	2.32	0.54
1:A:131:ALA:O	1:A:132:GLY:O	2.27	0.53
1:A:182:ARG:HD2	1:A:211:ALA:CB	2.38	0.52
1:A:332:TYR:HB3	1:A:335:HIS:HD2	1.74	0.52
1:A:1:ASP:OD2	1:A:108:LYS:NZ	2.43	0.52
1:A:61:ARG:NH2	1:A:82:ASP:OD2	2.27	0.51
1:A:283:ARG:HD2	1:A:326:PRO:CB	2.40	0.51
1:A:325:SER:HB2	1:A:326:PRO:CD	2.40	0.51
1:A:325:SER:HB2	1:A:326:PRO:HD2	1.92	0.50
1:A:81:HIS:HD2	3:A:508:HOH:O	1.95	0.49
1:A:56:MET:HG3	1:A:109:VAL:HG13	1.94	0.49
1:A:299:PRO:HD3	1:A:334:ASP:OD2	2.12	0.49
1:A:332:TYR:HB3	1:A:335:HIS:CD2	2.47	0.49
1:A:332:TYR:CE2	1:A:334:ASP:HB2	2.48	0.49
1:A:146:TYR:CG	1:A:147:PRO:HD2	2.48	0.49
1:A:62:ASP:O	1:A:75:GLY:HA2	2.13	0.48
1:A:132:GLY:O	1:A:133:GLN:CG	2.61	0.48
1:A:157:ILE:CG2	1:A:158:GLY:H	2.26	0.46
1:A:146:TYR:CD1	1:A:147:PRO:HD2	2.51	0.46
1:A:26:ASN:ND2	1:A:29:ARG:HE	2.13	0.46
1:A:292:ASN:HD22	1:A:294:ASP:H	1.64	0.46
1:A:292:ASN:HD21	1:A:295:THR:H	1.64	0.46
1:A:11:ARG:HH22	1:A:204:ASN:ND2	2.13	0.45
1:A:224:PRO:O	1:A:234:ASN:HA	2.16	0.45
1:A:390:ASP:O	1:A:391:LEU:C	2.55	0.44
1:A:81:HIS:HB2	1:A:125:LYS:HD3	1.99	0.44
1:A:319:TYR:OH	1:A:335:HIS:CD2	2.71	0.44
1:A:195:VAL:CG2	1:A:220:LEU:HB2	2.48	0.44
1:A:26:ASN:HD22	1:A:29:ARG:HH21	1.66	0.44
1:A:239:GLN:HG3	3:A:584:HOH:O	2.18	0.43
1:A:407:ASN:C	1:A:407:ASN:ND2	2.70	0.43
1:A:261:ARG:NE	1:A:261:ARG:HA	2.32	0.43
1:A:283:ARG:HD2	1:A:326:PRO:HB2	2.00	0.43
1:A:294:ASP:OD1	1:A:307:HIS:HD2	2.01	0.43
1:A:61:ARG:CD	1:A:84:ASN:HB3	2.49	0.42
1:A:155:ARG:HA	1:A:162:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ALA:HB1	1:A:214:SER:OG	2.19	0.42
1:A:232:TRP:CZ2	1:A:233:ARG:HD3	2.54	0.41
1:A:332:TYR:CD2	1:A:334:ASP:HB2	2.55	0.41
1:A:160:ASP:N	1:A:160:ASP:OD1	2.42	0.40
1:A:316:ARG:HH11	1:A:316:ARG:HD3	1.72	0.40
1:A:142:ASP:HA	1:A:143:PRO:HD2	1.72	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	411/418 (98%)	393 (96%)	14 (3%)	4 (1%)	18 10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	132	GLY
1	A	301	GLN
1	A	157	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	331/333 (99%)	307 (93%)	24 (7%)	16	11

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	TYR
1	A	42	GLN
1	A	61	ARG
1	A	65	SER
1	A	79	PHE
1	A	85	LYS
1	A	119	ASN
1	A	125	LYS
1	A	162	ASP
1	A	233	ARG
1	A	275	ASN
1	A	277	ASN
1	A	292	ASN
1	A	301	GLN
1	A	317	GLN
1	A	334	ASP
1	A	347	GLN
1	A	358	ARG
1	A	364	SER
1	A	367	SER
1	A	401	SER
1	A	403	SER
1	A	407	ASN
1	A	417	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	26	ASN
1	A	81	HIS
1	A	97	GLN
1	A	119	ASN
1	A	128	ASN
1	A	145	ASN
1	A	180	ASN
1	A	204	ASN

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Mol	Chain	Res	Type
1	A	240	GLN
1	A	264	ASN
1	A	277	ASN
1	A	292	ASN
1	A	307	HIS
1	A	311	GLN
1	A	317	GLN
1	A	335	HIS
1	A	347	GLN
1	A	366	HIS
1	A	388	ASN
1	A	407	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 2 ligands modelled in this entry, 2 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

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.