



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 09:12 am BST

PDB ID : 1UOK
Title : CRYSTAL STRUCTURE OF B. CEREUS OLIGO-1,6-GLUCOSIDASE
Authors : Watanabe, K.; Hata, Y.; Kizaki, H.; Katsube, Y.; Suzuki, Y.
Deposited on : 1998-07-28
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

<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

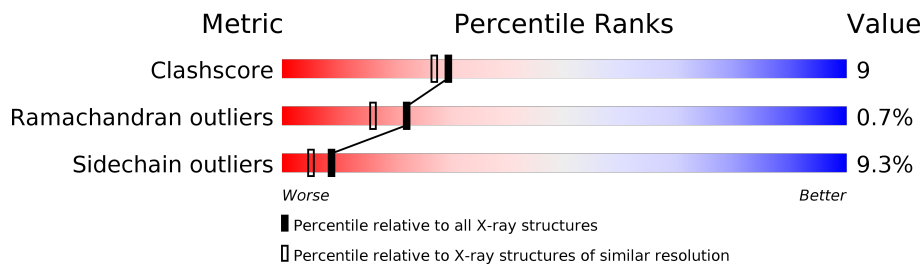
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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	558	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4867 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 OLIGO-1,6-GLUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	558	4646	2959	759	897	31	0	0	0

- Molecule 2 is water.

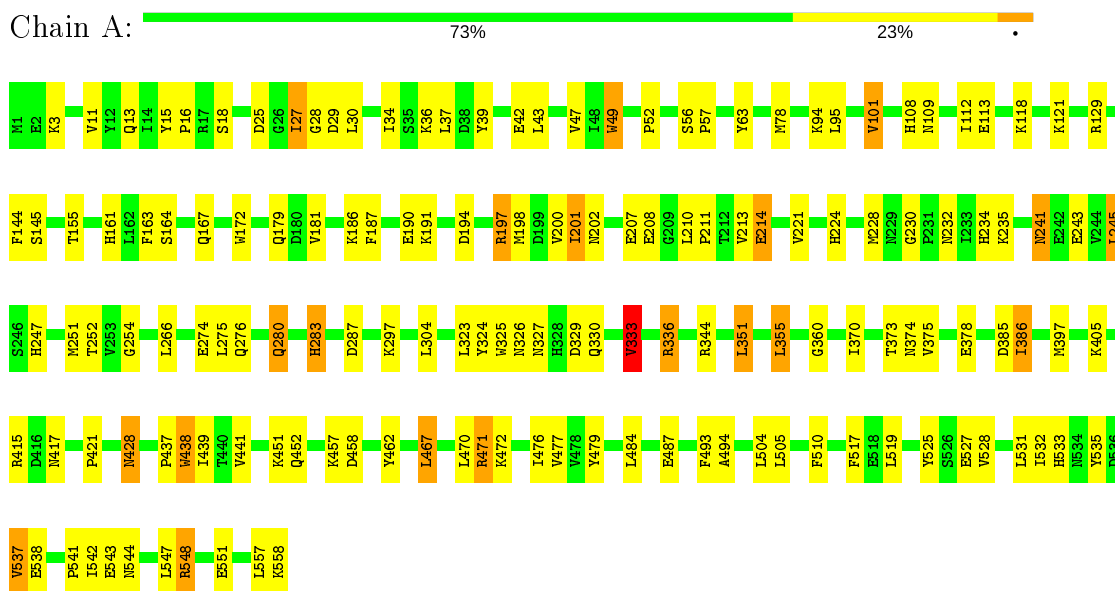
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	221	Total	O	0	0
			221	221		

3 Residue-property plots

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: OLIGO-1,6-GLUCOSIDASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	106.10Å 106.10Å 120.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	85.6 (8.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.192 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4867	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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	0.54	0/4766	0.80	8/6439 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	LEU	CA-CB-CG	6.96	131.30	115.30
1	A	197	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	25	ASP	CB-CG-OD1	5.82	123.53	118.30
1	A	538	GLU	N-CA-C	-5.57	95.96	111.00
1	A	197	ARG	N-CA-C	-5.39	96.45	111.00
1	A	15	TYR	N-CA-C	-5.13	97.15	111.00
1	A	333	VAL	CB-CA-C	-5.11	101.68	111.40
1	A	351	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4646	0	4422	86	0
2	A	221	0	0	4	0
All	All	4867	0	4422	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 9.

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)
1:A:373:THR:HG22	1:A:374:ASN:O	1.90	0.72
1:A:325:TRP:HB3	1:A:333:VAL:HG13	1.72	0.71
1:A:325:TRP:HB3	1:A:333:VAL:CG1	2.23	0.69
1:A:101:VAL:HG13	1:A:172:TRP:HZ2	1.58	0.68
1:A:287:ASP:OD2	1:A:336:ARG:HD3	1.96	0.66
1:A:18:SER:OG	1:A:438:TRP:HZ3	1.78	0.65
1:A:484:LEU:HD12	1:A:494:ALA:O	1.98	0.64
1:A:283:HIS:HE1	1:A:324:TYR:O	1.81	0.63
1:A:101:VAL:HG13	1:A:172:TRP:CZ2	2.34	0.62
1:A:533:HIS:HD2	1:A:535:TYR:O	1.82	0.61
1:A:241:ASN:HA	1:A:245:LEU:HB2	1.84	0.60
1:A:280:GLN:H	1:A:280:GLN:HE21	1.49	0.58
1:A:421:PRO:HB2	1:A:441:VAL:HG22	1.84	0.58
1:A:18:SER:OG	1:A:438:TRP:CZ3	2.57	0.57
1:A:385:ASP:OD2	1:A:415:ARG:HD3	2.05	0.56
1:A:234:HIS:HD2	1:A:274:GLU:OE1	1.88	0.56
1:A:375:VAL:H	1:A:417:ASN:HD22	1.55	0.54
1:A:11:VAL:HG22	1:A:47:VAL:HB	1.89	0.53
1:A:161:HIS:HD2	1:A:163:PHE:O	1.92	0.53
1:A:325:TRP:CG	1:A:333:VAL:HG11	2.43	0.52
1:A:207:GLU:OE2	1:A:211:PRO:HG2	2.10	0.52
1:A:525:TYR:CD2	1:A:528:VAL:HG23	2.45	0.51
1:A:213:VAL:HG22	1:A:221:VAL:HG21	1.94	0.50
1:A:344:ARG:NH2	1:A:370:ILE:O	2.45	0.50
1:A:548:ARG:HD3	1:A:551:GLU:OE1	2.11	0.50
1:A:519:LEU:HD22	1:A:542:ILE:HG13	1.95	0.49
1:A:144:PHE:O	1:A:145:SER:HB2	2.13	0.49
1:A:537:VAL:HG13	1:A:548:ARG:HH12	1.78	0.49
1:A:280:GLN:HE21	1:A:280:GLN:N	2.10	0.48
1:A:280:GLN:H	1:A:280:GLN:NE2	2.11	0.48
1:A:541:PRO:HB2	1:A:543:GLU:HG2	1.94	0.48
1:A:329:ASP:HA	1:A:415:ARG:HG2	1.95	0.48
1:A:201:ILE:HD11	1:A:254:GLY:HA3	1.95	0.47
1:A:161:HIS:CE1	2:A:710:HOH:O	2.66	0.47
1:A:36:LYS:O	1:A:39:TYR:HB3	2.15	0.47
1:A:326:ASN:HB2	2:A:674:HOH:O	2.13	0.47
1:A:214:GLU:CD	1:A:214:GLU:H	2.18	0.47
1:A:386:ILE:HG13	1:A:386:ILE:H	1.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:MET:HB2	1:A:201:ILE:HG12	1.97	0.47
1:A:251:MET:HA	1:A:276:GLN:HE22	1.80	0.46
1:A:533:HIS:CD2	1:A:535:TYR:O	2.65	0.46
1:A:528:VAL:HG22	1:A:557:LEU:CD2	2.46	0.46
1:A:476:ILE:HD13	1:A:504:LEU:HG	1.97	0.46
1:A:360:GLY:O	1:A:471:ARG:NH2	2.48	0.46
1:A:528:VAL:HG22	1:A:557:LEU:HD22	1.97	0.46
1:A:232:ASN:HD22	1:A:235:LYS:NZ	2.14	0.46
1:A:201:ILE:HD11	1:A:254:GLY:CA	2.45	0.46
1:A:224:HIS:O	1:A:228:MET:HB2	2.16	0.45
1:A:3:LYS:HG2	1:A:479:TYR:CZ	2.52	0.45
1:A:326:ASN:ND2	1:A:333:VAL:HG22	2.31	0.45
1:A:52:PRO:HD3	1:A:63:TYR:CZ	2.51	0.45
1:A:49:TRP:CE2	1:A:197:ARG:HG3	2.52	0.44
1:A:243:GLU:O	1:A:247:HIS:CE1	2.71	0.44
1:A:325:TRP:HB3	1:A:333:VAL:HG11	1.99	0.44
1:A:187:PHE:O	1:A:191:LYS:HG2	2.18	0.44
1:A:13:GLN:HG3	1:A:49:TRP:CD2	2.53	0.44
1:A:101:VAL:CG1	1:A:172:TRP:HZ2	2.27	0.43
1:A:94:LYS:HB3	1:A:194:ASP:HB2	2.01	0.43
1:A:108:HIS:O	1:A:112:ILE:HG12	2.17	0.43
1:A:161:HIS:HE1	2:A:710:HOH:O	2.00	0.43
1:A:198:MET:HB2	1:A:201:ILE:CG1	2.48	0.43
1:A:251:MET:HB2	1:A:276:GLN:HE22	1.83	0.43
1:A:27:ILE:HD12	1:A:28:GLY:O	2.19	0.43
1:A:16:PRO:HD2	2:A:631:HOH:O	2.18	0.43
1:A:327:ASN:OD1	1:A:330:GLN:HG2	2.19	0.43
1:A:78:MET:HB2	1:A:78:MET:HE2	1.89	0.43
1:A:118:LYS:HE3	1:A:155:THR:HB	2.01	0.42
1:A:101:VAL:HG21	1:A:181:VAL:HG13	2.01	0.42
1:A:36:LYS:HA	1:A:36:LYS:HD3	1.71	0.42
1:A:527:GLU:HB3	1:A:558:LYS:HA	2.01	0.42
1:A:121:LYS:HE3	1:A:121:LYS:HB2	1.88	0.42
1:A:457:LYS:HA	1:A:462:TYR:CD2	2.56	0.41
1:A:186:LYS:O	1:A:190:GLU:HG2	2.20	0.41
1:A:437:PRO:HB2	1:A:439:ILE:O	2.20	0.41
1:A:252:THR:H	1:A:276:GLN:NE2	2.18	0.41
1:A:56:SER:HA	1:A:57:PRO:HD3	1.95	0.41
1:A:202:ASN:O	1:A:228:MET:O	2.39	0.41
1:A:373:THR:CG2	1:A:374:ASN:N	2.83	0.41
1:A:451:LYS:HD3	1:A:451:LYS:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:LEU:HD12	1:A:467:LEU:HA	1.94	0.41
1:A:47:VAL:HG21	1:A:251:MET:HE3	2.03	0.41
1:A:30:LEU:O	1:A:34:ILE:HG13	2.21	0.40
1:A:467:LEU:HD13	1:A:532:ILE:HD13	2.03	0.40
1:A:517:PHE:O	1:A:544:ASN:HA	2.22	0.40
1:A:164:SER:H	1:A:167:GLN:HE21	1.69	0.40
1:A:109:ASN:O	1:A:113:GLU:HG2	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	556/558 (100%)	528 (95%)	24 (4%)	4 (1%)	22 16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	GLU
1	A	230	GLY
1	A	428	ASN
1	A	200	VAL

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	508/508 (100%)	461 (91%)	47 (9%)	9 5

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	29	ASP
1	A	37	LEU
1	A	42	GLU
1	A	43	LEU
1	A	49	TRP
1	A	95	LEU
1	A	101	VAL
1	A	129	ARG
1	A	179	GLN
1	A	201	ILE
1	A	208	GLU
1	A	210	LEU
1	A	241	ASN
1	A	245	LEU
1	A	266	LEU
1	A	275	LEU
1	A	280	GLN
1	A	283	HIS
1	A	297	LYS
1	A	304	LEU
1	A	323	LEU
1	A	333	VAL
1	A	336	ARG
1	A	351	LEU
1	A	355	LEU
1	A	378	GLU
1	A	386	ILE
1	A	397	MET
1	A	405	LYS
1	A	428	ASN
1	A	438	TRP
1	A	452	GLN
1	A	458	ASP
1	A	467	LEU
1	A	470	LEU
1	A	471	ARG
1	A	472	LYS

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Mol	Chain	Res	Type
1	A	477	VAL
1	A	487	GLU
1	A	493	PHE
1	A	505	LEU
1	A	510	PHE
1	A	531	LEU
1	A	537	VAL
1	A	547	LEU
1	A	548	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	150	GLN
1	A	161	HIS
1	A	167	GLN
1	A	224	HIS
1	A	226	HIS
1	A	232	ASN
1	A	234	HIS
1	A	241	ASN
1	A	247	HIS
1	A	276	GLN
1	A	280	GLN
1	A	283	HIS
1	A	321	ASN
1	A	326	ASN
1	A	330	GLN
1	A	390	ASN
1	A	417	ASN
1	A	428	ASN
1	A	452	GLN
1	A	455	GLN
1	A	473	ASN
1	A	533	HIS
1	A	539	ASN

5.3.3 RNA

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](#)

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.