

Full wwPDB X-ray Structure Validation Report (i)

Aug 10, 2021 – 10:07 am BST

PDB ID : 7A0T

Title : Crystal structure of kievitone hydratase from Nectria haematococca (P21 SG)

Authors: Pavkov-Keller, T.; Gruber, K.

Deposited on : 2020-08-10

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ Xtriage (Phenix) & : & 1.13 \\ & EDS & : & \textbf{FAILED} \end{array}$

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)

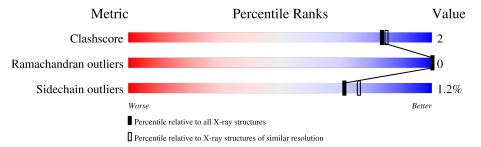
Validation Pipeline (wwPDB-VP) : 2.23.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)



2 Entry composition (i)

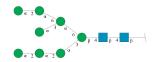
There are 5 unique types of molecules in this entry. The entry contains 5866 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CrtC domain-containing protein.

Mol	Chain	Residues	${f Atoms}$		ZeroOcc	AltConf	Trace			
1	Δ	325	Total C N O		2	0				
1	Λ	329	2590	1654	420	516	U			
1	D	326	Total	С	N	О	0	1	0	
1	Б	320	2588	1653	419	516	U	1	0	

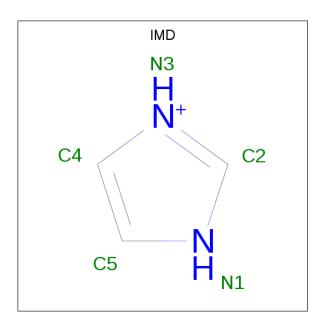
• Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	С	10	Total 116 6	C N 64 2		0	0	0
2	D	10	Total 116 6	C N 64 2	O 50	0	0	0

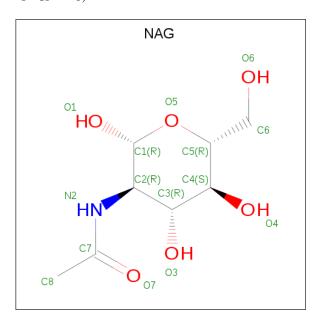
• Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 5 3 2	0	0
3	В	1	Total C N 5 3 2	0	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	В	1	Total 14	C 8	N 1	O 5	0	0



• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	192	Total O 192 192	0	0
5	В	240	Total O 240 240	0	0

 ${\tt SEQUENCE-PLOTS\ INFOmissing INFO}$



3 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	51.43Å 79.79Å 103.18Å	Depositor	
a, b, c, α , β , γ	90.00° 100.68° 90.00°	Depositor	
Resolution (Å)	49.00 - 2.00	Depositor	
% Data completeness	99.3 (49.00-2.00)	Depositor	
(in resolution range)	,	•	
R_{merge}	0.10	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.65 (at 2.00Å)	Xtriage	
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor	
R, R_{free}	0.176 , 0.209	Depositor	
Wilson B-factor (A^2)	30.9	Xtriage	
Anisotropy	0.171	Xtriage	
L-test for twinning ² $ < L > = 0.49, < L^2 > = 0.33 $		Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage wwPDB-VP	
Total number of atoms	ber of atoms 5866		
Average B, all atoms (\mathring{A}^2)	34.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, IMD, BMA, MAN

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.45	0/2669	0.57	0/3646	
1	В	0.44	0/2668	0.57	0/3646	
All	All	0.45	0/5337	0.57	0/7292	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	2590	0	2442	15	0
1	В	2588	0	2437	11	0
2	С	116	0	97	0	0
2	D	116	0	97	1	0
3	A	5	0	5	0	0
3	В	5	0	5	2	0
4	В	14	0	13	1	0
5	A	192	0	0	3	0
5	В	240	0	0	0	0
All	All	5866	0	5096	25	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 2.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		$\operatorname{distance}\left(\mathrm{\AA}\right)$	overlap (Å)
1:B:348:VAL:HG21	2:D:8:MAN:H62	1.60	0.82
1:A:24:LYS:NZ	5:A:705:HOH:O	2.32	0.62
1:A:128:GLU:HB2	1:A:135[A]:LYS:HG3	1.82	0.60
1:A:347:ASP:OD1	1:A:348:VAL:N	2.35	0.59
1:A:309:VAL:O	5:A:701:HOH:O	2.18	0.52
1:A:224:LEU:HB2	1:A:233:ILE:HB	1.94	0.50
1:B:127:SER:OG	1:B:132:ASN:HA	2.13	0.49
1:A:131:ASP:OD2	1:A:134:SER:OG	2.31	0.47
1:A:301:SER:HA	1:A:322:ILE:HG22	1.97	0.47
1:B:340:GLU:OE1	3:B:502:IMD:H4	2.14	0.46
1:A:151:TYR:HA	1:A:182:LYS:O	2.16	0.46
1:A:142:HIS:O	1:A:146:THR:OG1	2.35	0.45
1:A:275:GLU:OE2	1:A:282:THR:OG1	2.34	0.45
1:B:301:SER:HA	1:B:322:ILE:HG22	1.98	0.44
1:B:275:GLU:HG3	1:B:282:THR:HG22	2.00	0.44
1:A:179:PRO:HB3	1:A:204:TRP:CZ3	2.54	0.42
1:A:272:ARG:NH1	5:A:708:HOH:O	2.38	0.42
1:B:324:PHE:CZ	1:B:335:GLY:HA3	2.55	0.42
1:B:60:TRP:CD2	3:B:502:IMD:H5	2.55	0.42
1:A:34:LYS:HD3	1:A:34:LYS:HA	1.73	0.41
1:B:112:ASN:ND2	4:B:501:NAG:O7	2.53	0.41
1:A:172:LEU:HD21	1:B:44:VAL:HB	2.03	0.40
1:B:347:ASP:OD1	1:B:348:VAL:N	2.55	0.40
1:A:135[A]:LYS:NZ	1:A:152:ASP:OD1	2.37	0.40
1:B:102:GLN:HB2	1:B:308:LEU:HD23	2.02	0.40

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	Perce	$_{ m ntiles}$
1	A	325/348~(93%)	314 (97%)	11 (3%)	0	100	100
1	В	325/348~(93%)	309 (95%)	16 (5%)	0	100	100
All	All	$650/696 \ (93\%)$	623 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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	283/296~(96%)	278 (98%)	5 (2%)	59 63
1	В	283/296 (96%)	280 (99%)	3 (1%)	73 78
All	All	566/592 (96%)	558 (99%)	8 (1%)	71 72

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	135[A]	LYS
1	A	135[B]	LYS
1	A	206	ASP
1	A	296	ASP
1	В	123	ASN
1	В	151	TYR
1	В	331	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

4.3.3 RNA (i)

There are no RNA molecules in this entry.



4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

20 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

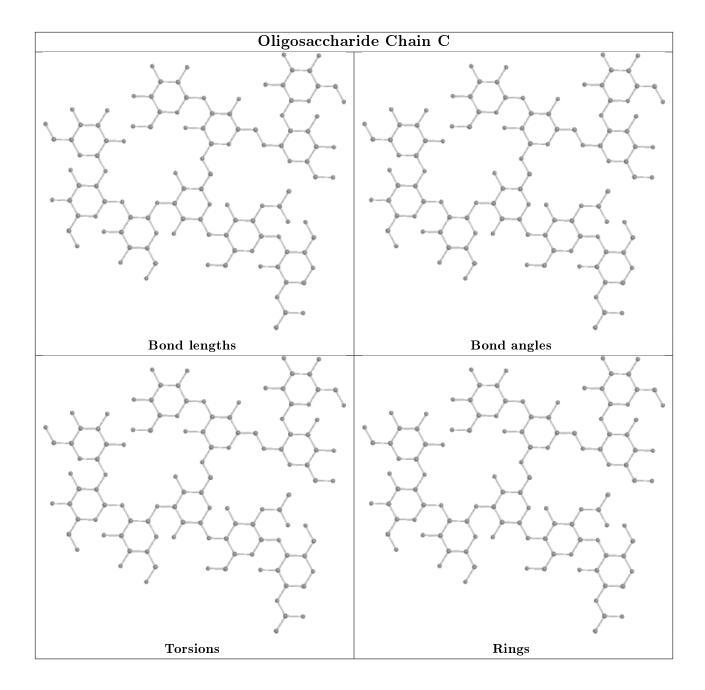
There are no torsion outliers.

There are no ring outliers.

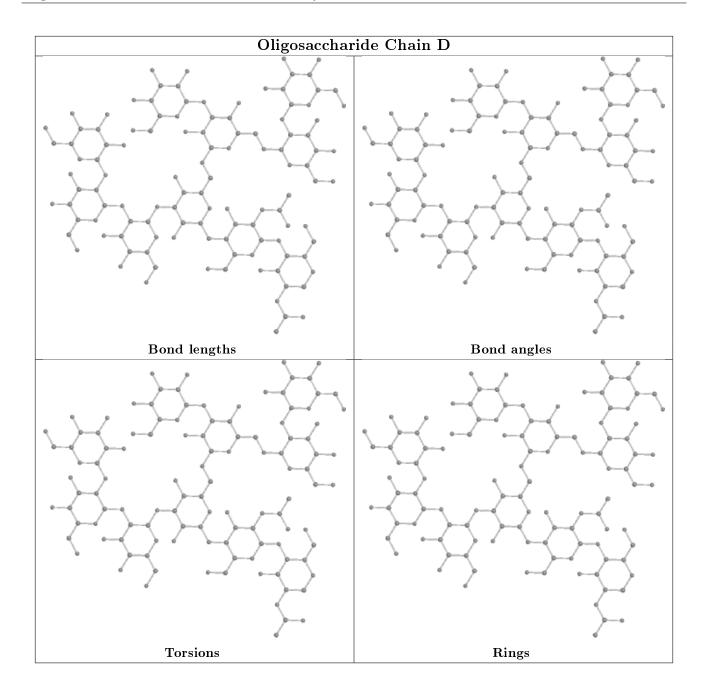
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









4.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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.



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

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

5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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

