

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 15, 2023 – 07:16 PM EDT

PDB ID	:	8E0R
Title	:	Crystal structure of mouse APCDD1 in P21 space group
Authors	:	Hsieh, F.L.; Chang, T.H.; Gabelli, S.B.; Nathans, J.
Deposited on		
Resolution	:	1.95  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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

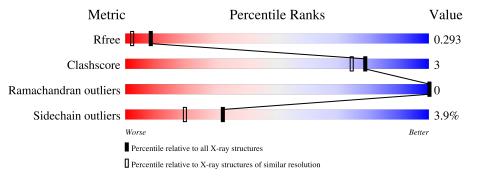
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 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 1.95 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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 of 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 <=5%

Mol	Chain	Length	Quality of chain		
1	А	468	81%	8%	11%
1	В	468	76%	10% •	13%



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7140 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	418	Total 3389	C 2140	11	O 609	S 22	0	3	0
1	В	405	Total 3307	C 2096	N 604	0 587	S 20	0	2	0

• Molecule 1 is a protein called Protein APCDD1.

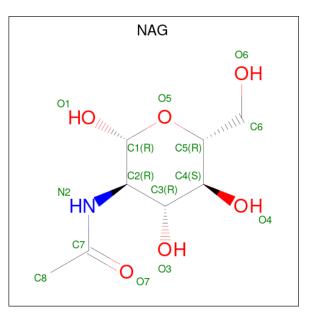
Chain	Residue	Modelled	Actual	Comment	Reference
А	24	GLU	-	expression tag	UNP Q3U128
А	25	THR	-	expression tag	UNP Q3U128
А	26	GLY	-	expression tag	UNP Q3U128
А	483	THR	-	expression tag	UNP Q3U128
А	484	HIS	-	expression tag	UNP Q3U128
А	485	HIS	-	expression tag	UNP $Q3U128$
А	486	HIS	-	expression tag	UNP Q3U128
А	487	HIS	-	expression tag	UNP Q3U128
A	488	HIS	-	expression tag	UNP Q3U128
Α	489	HIS	-	expression tag	UNP Q3U128
A	490	HIS	-	expression tag	UNP Q3U128
А	491	HIS	-	expression tag	UNP Q3U128
В	24	GLU	-	expression tag	UNP Q3U128
В	25	THR	-	expression tag	UNP Q3U128
В	26	GLY	-	expression tag	UNP Q3U128
В	483	THR	-	expression tag	UNP $Q3U128$
В	484	HIS	-	expression tag	UNP Q3U128
В	485	HIS	-	expression tag	UNP $Q3U128$
В	486	HIS	-	expression tag	UNP Q3U128
В	487	HIS	-	expression tag	UNP Q3U128
В	488	HIS	-	expression tag	UNP Q3U128
В	489	HIS	-	expression tag	UNP Q3U128
В	490	HIS	-	expression tag	UNP Q3U128
В	491	HIS	-	expression tag	UNP Q3U128

There are 24 discrepancies between the modelled and reference sequences:





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



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

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	194	Total O 194 194	0	0
3	В	180	Total O 180 180	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

Chain A:	81%	8% 11%
0LU TTRR CTRR CLEU LEU LEU LEU LEU LEU LEU ARS SER SER SER ARG PRO ARG	SEK LUU GLU CLNS SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	A176 P177 D184 S194 T199 F204 F204 F204 F219 F219 F219 F215
V243 F244 N261 H262 A263 A263 A263 A265 A284 A284 A285 A298 A298 A298 A298	A335 F3339 F3339 F3339 F3378 F3378 F3378 F3378 F3378 F3378 F3378 F3378 F3378 F3378 F3378 F3378 F3378 F3378 F4378 F413 F413 F413 F413 F413 F413 F413 F413	1417 1424 1424 1424 1451 1421 1421 1421 1421
THR HIS HIS HIS HIS HIS HIS HIS		
• Molecule 1: Prote	in APCDD1	
Chain B:	76%	10% • 13%
GLU THR GLY GLY CLY LEU HIS PRO ARG SER HIS PRO ARG	SEK LUU LUS CLU TRP ALA ALA ALA ALA ALA ALA ALA BR GLU BR BR BR BR BR BR BR BR BR BR BR BR BR	R114 R129 E157 E157 E157 R163 R165 R165 C175 C178 C178 V181
D184           1	D224 H225 L226 L226 H312 H312 H322 F339 F339 F339 F339 F339 F339 F339 F	417 417 417 417 417 417 414 634 634 640 7406 7406 7406 7406 7406 7406 7411 747 747 747 747 747 747 7411
1424 1425 1421 1431 1431 1431 1431 1435 1465 1465 1468	SER PRO ALK ALK CUU CUU CUU CUU CUU CUU CUU CUU CUU CU	

• Molecule 1: Protein APCDD1



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	49.86Å 144.13Å 64.38Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $99.52^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	34.00 - 1.95	Depositor
	34.36 - 1.95	EDS
% Data completeness	76.6(34.00-1.95)	Depositor
(in resolution range)	76.3(34.36-1.95)	EDS
R <sub>merge</sub>	0.14	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.11 (at 1.95 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
$R, R_{free}$	0.209 , $0.247$	Depositor
It, Itfree	0.264 , $0.293$	DCC
$R_{free}$ test set	2407 reflections $(4.82%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	32.0	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.38 , $40.1$	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.52, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7140	wwPDB-VP
Average B, all atoms $(Å^2)$	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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	Chain	Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.64	0/3498	0.79	1/4748~(0.0%)	
1	В	0.71	3/3416~(0.1%)	0.82	7/4637~(0.2%)	
All	All	0.67	3/6914~(0.0%)	0.81	8/9385~(0.1%)	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	368[A]	HIS	C-O	10.92	1.44	1.23
1	В	368[B]	HIS	C-O	10.92	1.44	1.23
1	В	368[C]	HIS	C-O	10.92	1.44	1.23

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	В	368[A]	HIS	CA-C-O	6.64	134.04	120.10
1	В	368[B]	HIS	CA-C-O	6.64	134.04	120.10
1	В	368[C]	HIS	CA-C-O	6.64	134.04	120.10
1	В	368[A]	HIS	O-C-N	-6.49	112.31	122.70
1	В	368[B]	HIS	O-C-N	-6.49	112.31	122.70
1	В	368[C]	HIS	O-C-N	-6.49	112.31	122.70
1	В	455	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	А	244	PHE	CB-CA-C	-5.80	98.79	110.40

All (8) bond angle outliers are listed below:

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	А	3389	0	3244	17	0
1	В	3307	0	3169	22	3
2	А	42	0	39	0	0
2	В	28	0	26	0	0
3	А	194	0	0	2	0
3	В	180	0	0	2	0
All	All	7140	0	6478	37	3

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 3.

All (37) 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:403:ASP:OD1	1:A:405:THR:HG23	1.91	0.70
1:A:298:GLN:OE1	3:A:601:HOH:O	2.09	0.70
1:A:368[A]:HIS:CD2	1:A:405:THR:HG21	2.30	0.66
1:B:339:PHE:HB3	1:B:378:THR:HG21	1.83	0.61
1:B:224:ASP:OD2	3:B:601:HOH:O	2.15	0.60
1:B:369:MET:H	1:B:405:THR:HG22	1.68	0.59
1:A:339:PHE:HB3	1:A:378:THR:HG21	1.85	0.58
1:B:219:PRO:HD2	1:B:225:HIS:O	2.06	0.55
1:A:101:ASN:HB2	1:A:127:LYS:HE2	1.90	0.51
1:A:225[B]:HIS:CE1	1:A:262:HIS:H	2.29	0.51
1:B:129:ARG:NH2	3:B:604:HOH:O	2.32	0.50
1:B:157:GLU:CD	1:B:157:GLU:H	2.14	0.50
1:A:219:PRO:HB2	1:A:222:SER:HB3	1.94	0.49
1:B:451:ARG:NH1	1:B:454:LYS:HD2	2.27	0.48
1:B:56:LEU:HD11	1:B:312:HIS:HB2	1.94	0.48
1:A:263:ALA:HA	1:B:431:THR:O	2.13	0.48
1:B:403:ASP:OD1	1:B:405:THR:HG23	2.14	0.48
1:B:322:TRP:HZ2	1:B:366:VAL:HG22	1.80	0.47
1:B:425:PHE:HD2	1:B:437:LEU:HD11	1.81	0.46
1:A:199:THR:HB	1:A:204:PHE:HB3	1.98	0.46
1:B:76:HIS:HE2	1:B:94:SER:HG	1.62	0.46

Continued on next page...



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:HD3	1:A:284:LYS:O	2.17	0.44
1:B:157:GLU:CD	1:B:157:GLU:N	2.71	0.44
1:A:285:ALA:HB2	1:B:225:HIS:NE2	2.32	0.44
1:A:405:THR:HA	1:A:417:LEU:HD12	2.01	0.43
1:B:162:GLN:O	1:B:165:ARG:HG2	2.19	0.43
1:A:225[B]:HIS:CE1	1:A:261:ASN:HA	2.55	0.42
1:B:164:SER:HB3	1:B:181:TRP:HB2	2.01	0.42
1:B:199:THR:HB	1:B:204:PHE:HB3	2.02	0.42
1:A:219:PRO:HA	3:A:672:HOH:O	2.20	0.41
1:B:178:GLY:O	1:B:180:PRO:HD3	2.21	0.41
1:A:176:ALA:HB1	1:A:177:PRO:CD	2.50	0.41
1:A:368[A]:HIS:CE1	1:A:370:LYS:HG3	2.56	0.41
1:B:112:SER:OG	1:B:114:ARG:HG2	2.21	0.41
1:B:226:LEU:O	1:B:259:ASN:HB3	2.21	0.41
1:A:159:VAL:O	1:A:163:LEU:HB2	2.20	0.40

Continued from previous page...

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:GLN:NE2	$1:B:406:HIS:CD2[1_556]$	1.95	0.25
1:B:224:ASP:OD2	$1:B:354:SER:OG[1_455]$	2.11	0.09
1:B:191:GLN:NE2	$1:B:406:HIS:NE2[1_556]$	2.13	0.07

### 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	Percer	ntiles
1	А	415/468 (89%)	391 (94%)	24~(6%)	0	100	100
1	В	400/468~(86%)	383~(96%)	17 (4%)	0	100	100
All	All	815/936~(87%)	774 (95%)	41 (5%)	0	100	100



There are no Ramachandran outliers to report.

#### 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	А	369/411~(90%)	353~(96%)	16 (4%)	29 16
1	В	360/411 (88%)	348~(97%)	12 (3%)	38 26
All	All	729/822~(89%)	701 (96%)	28~(4%)	32 21

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	86	SER
1	А	129	ARG
1	А	184	ASP
1	А	194	SER
1	А	200	LYS
1	А	243	VAL
1	А	244	PHE
1	А	306	VAL
1	А	335	LYS
1	А	405	THR
1	А	410	CYS
1	А	411	VAL
1	А	413	LEU
1	А	424	ILE
1	А	451	ARG
1	А	469	SER
1	В	60	HIS
1	В	64	ARG
1	В	86	SER
1	В	114	ARG
1	В	157	GLU
1	В	163	LEU
1	В	175	LEU
1	В	184	ASP
1	В	299	ARG

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type
1	В	355	LYS
1	В	405	THR
1	В	424	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	107	GLN
1	А	402	GLN
1	В	60	HIS
1	В	107	GLN
1	В	328	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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
Mol Type	Unain	ii nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
2	NAG	А	501	1	14,14,15	0.28	0	$17,\!19,\!21$	1.32	1 (5%)



Mal	Mol Type Chain		Res	Link	Bond lengths			Bond angles		
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	NAG	В	502	1	14,14,15	0.54	0	$17,\!19,\!21$	1.42	4 (23%)
2	NAG	В	501	1	14,14,15	0.32	0	17,19,21	1.28	1 (5%)
2	NAG	А	503	1	14,14,15	0.45	0	17,19,21	0.97	2 (11%)
2	NAG	А	502	1	14,14,15	0.34	0	17,19,21	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	А	501	1	-	2/6/23/26	0/1/1/1
2	NAG	В	502	1	-	0/6/23/26	0/1/1/1
2	NAG	В	501	1	-	1/6/23/26	0/1/1/1
2	NAG	А	503	1	-	0/6/23/26	0/1/1/1
2	NAG	А	502	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	501	NAG	C1-O5-C5	4.79	118.68	112.19
2	В	501	NAG	C1-O5-C5	3.73	117.25	112.19
2	В	502	NAG	O5-C5-C6	2.81	111.62	107.20
2	В	502	NAG	C4-C3-C2	-2.59	107.22	111.02
2	В	502	NAG	C3-C4-C5	-2.52	105.73	110.24
2	А	503	NAG	O4-C4-C3	-2.33	104.97	110.35
2	В	502	NAG	O5-C5-C4	-2.15	105.59	110.83
2	А	503	NAG	C1-C2-N2	2.06	114.00	110.49

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	501	NAG	C4-C5-C6-O6
2	А	501	NAG	O5-C5-C6-O6
2	В	501	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.



## 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

