

wwPDB X-ray Structure Validation Summary Report (i)

Dec 19, 2023 – 03:06 PM EST

PDB ID : 1J37

Title : Crystal Structure of Drosophila AnCE

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Deposited on : 2003-01-20

Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (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)

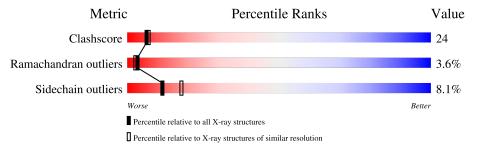
Validation Pipeline (wwPDB-VP) : 2.36

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 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain				
1	A	607	54%	38%	6% •		
1	В	607	55%	38%	6% •		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9830 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 angiotensin converting enzyme.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	598	Total 4900	C 3135	N 819	O 926	S 20	154	0	0
1	В	598	Total 4900	C 3135	N 819	O 926	S 20	154	0	0

There are 16 discrepancies between the modelled and reference sequences:

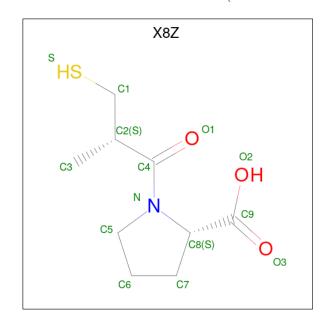
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ARG	GLY	conflict	UNP Q10714
A	53	ALA	ASN	conflict	UNP Q10714
A	607	ILE	THR	conflict	UNP Q10714
A	616	HIS	_	expression tag	UNP Q10714
A	617	HIS	-	expression tag	UNP Q10714
A	618	HIS	-	expression tag	UNP Q10714
A	619	HIS	-	expression tag	UNP Q10714
A	620	HIS	-	expression tag	UNP Q10714
В	51	ARG	GLY	conflict	UNP Q10714
В	53	ALA	ASN	conflict	UNP Q10714
В	607	ILE	THR	conflict	UNP Q10714
В	616	HIS	-	expression tag	UNP Q10714
В	617	HIS	-	expression tag	UNP Q10714
В	618	HIS	-	expression tag	UNP Q10714
В	619	HIS	-	expression tag	UNP Q10714
В	620	HIS	-	expression tag	UNP Q10714

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0



 \bullet Molecule 3 is L-CAPTOPRIL (three-letter code: X8Z) (formula: $\mathrm{C_9H_{15}NO_3S}).$



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
2	Λ	1	Total	С	N	О	S	0	0	
3	3 A	1	14	9	1	3	1	0		
9	D	1	Total	С	N	О	S	0	0	
3	Б	1	14	9	1	3	1		0	

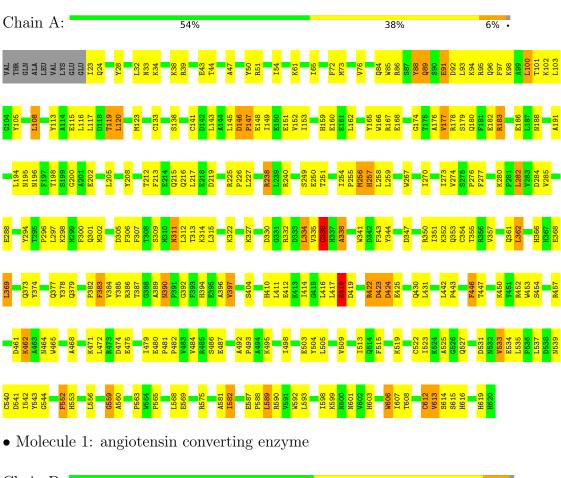


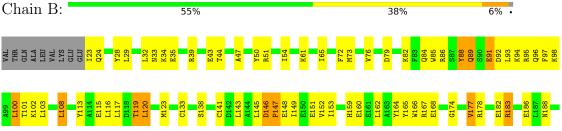
3 Residue-property plots (i)

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.

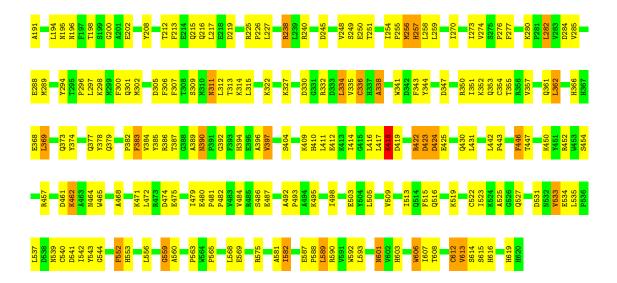
Note EDS was not executed.

• Molecule 1: angiotensin converting enzyme











4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	94.91Å 121.22Å 94.74Å	Depositor	
a, b, c, α , β , γ	90.00° 99.39° 90.00°	Depositor	
Resolution (Å)	20.00 - 2.40	Depositor	
% Data completeness	(Not available) (20.00-2.40)	Depositor	
(in resolution range)	(1100 available) (20.00 2.10)		
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	CNS	Depositor	
R, R_{free}	0.241 , 0.283	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	9830	wwPDB-VP	
Average B, all atoms (Å ²)	28.0	wwPDB-VP	



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: X8Z, ZN

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.46	0/5031	0.67	1/6814~(0.0%)	
1	В	0.46	0/5031	0.68	0/6814	
All	All	0.46	0/10062	0.68	1/13628 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	A	336	CYS	CA-CB-SG	-5.93	103.33	114.00

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	4900	0	4696	222	0
1	В	4900	0	4696	231	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
3	A	14	0	13	0	0
3	В	14	0	13	0	0
All	All	9830	0	9418	450	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 24.

The worst 5 of 450 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:533:VAL:HG22	1:A:534:GLU:H	1.20	1.06
1:B:533:VAL:HG22	1:B:534:GLU:H	1.21	1.04
1:B:418:LYS:HE3	1:B:418:LYS:H	1.29	0.95
1:A:347:ASP:H	1:A:379:GLN:HE22	1.14	0.91
1:A:418:LYS:HE3	1:A:418:LYS:H	1.34	0.91

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	596/607 (98%)	532 (89%)	42 (7%)	22 (4%)	3 2
1	В	596/607 (98%)	535 (90%)	40 (7%)	21 (4%)	3 3
All	All	1192/1214 (98%)	1067 (90%)	82 (7%)	43 (4%)	3 3

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO
1	A	256	MET
1	A	257	HIS
1	A	423	ASP
1	A	424	ASP



5.3.2Protein 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	522/530 (98%)	480 (92%)	42 (8%)	12	18
1	В	522/530 (98%)	479 (92%)	43 (8%)	11	17
All	All	1044/1060 (98%)	959 (92%)	85 (8%)	11	18

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	314	LYS
1	В	461	ASP
1	В	336	CYS
1	В	404	SER
1	В	537	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	31	ASN
1	В	610	ASN
1	В	195	ASN
1	В	601	ASN
1	В	464	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	Trme	Type Chain Res L		Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	X8Z	В	802	2	14,14,14	1.20	1 (7%)	18,19,19	0.98	1 (5%)
3	X8Z	A	801	2	14,14,14	1.05	1 (7%)	18,19,19	0.97	1 (5%)

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
3	X8Z	В	802	2	-	0/14/24/24	0/1/1/1
3	X8Z	A	801	2	=	0/14/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
3	В	802	X8Z	O1-C4	2.94	1.27	1.22
3	A	801	X8Z	O1-C4	2.62	1.27	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
3	В	802	X8Z	C6-C7-C8	2.15	108.67	104.18
3	A	801	X8Z	C6-C7-C8	2.11	108.60	104.18

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 (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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

