



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:26 PM UTC

PDB ID : 1J38 / pdb_00001j38
Title : Crystal Structure of Drosophila AnCE
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Deposited on : 2003-01-20
Resolution : 2.60 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

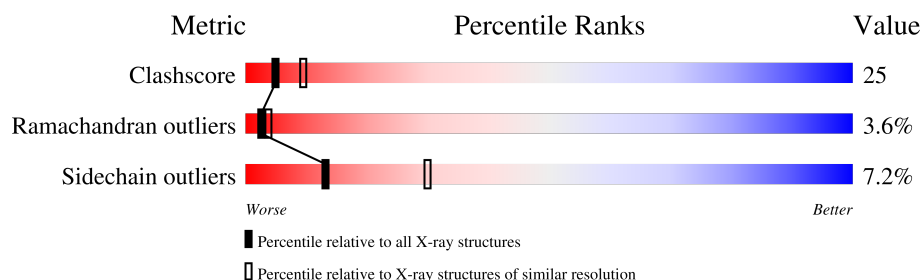
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	607	 53% 36% 9% ..
1	B	607	 54% 35% 9% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9806 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	C	N	O	S	154	0	0
			4900	3135	819	926	20			
1	B	598	Total	C	N	O	S	154	0	0
			4900	3135	819	926	20			

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
B	51	ARG	GLY	conflict	UNP Q10714
B	53	ALA	ASN	conflict	UNP Q10714
B	607	ILE	THR	conflict	UNP Q10714
B	616	HIS	-	expression tag	UNP Q10714
B	617	HIS	-	expression tag	UNP Q10714
B	618	HIS	-	expression tag	UNP Q10714
B	619	HIS	-	expression tag	UNP Q10714
B	620	HIS	-	expression tag	UNP Q10714

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	O 2	0	0
3	B	2	Total 2	O 2	0	0

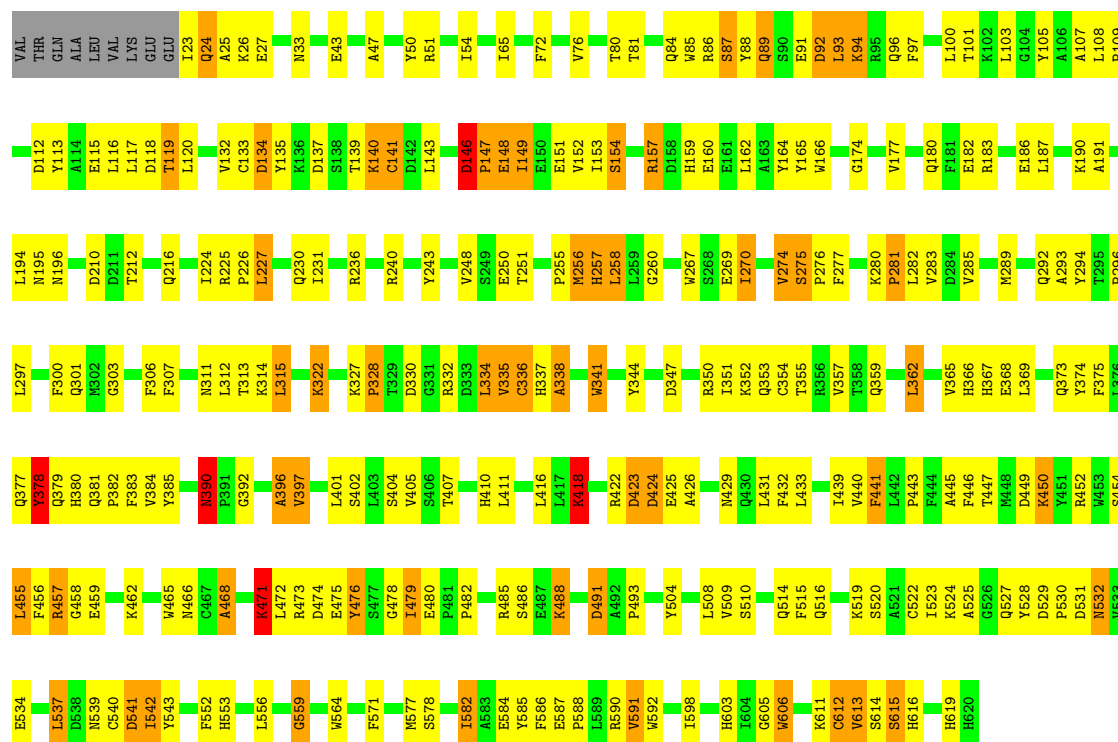
3 Residue-property plots [i](#)

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.

Note EDS was not executed.

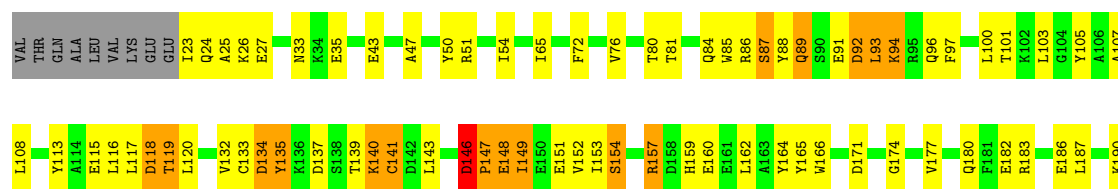
- Molecule 1: angiotensin converting enzyme

Chain A:  53% 36% 9% ..



- Molecule 1: angiotensin converting enzyme

Chain B:  54% 35% 9% ..



A191	F306	V384	W465	N539
L194	F307	Y385	N466	C540
N195	M310	K390	A467	D541
N196	N311	F391	F469	I542
D210	L312	W392	W470	Y543
Q216	T313	A396	K471	F552
I224	K314	V397	L472	H553
R225	L315	L401	R473	L556
P226	K322	S402	D474	G559
L227	K327	V405	Y475	W564
Q230	P328	S406	S477	F571
I231	T329	T407	G478	M577
R236	D330	H410	L479	S578
Y243	G331	L411	E480	I582
T251	R332	L416	P481	A583
I254	D333	L417	P482	E584
P255	L334	K418	R485	Y585
M256	V335	R422	S486	F586
H257	C336	D423	E487	E587
L258	H337	D424	K488	P588
L259	A338	E425	D491	L589
G260	W341	A426	A492	R590
W267	Y344	N429	P493	V591
S268	D347	G430	Y504	W592
E269	R350	L431	L508	H603
I270	I351	F432	V509	T604
V274	K352	L433	S510	G605
S275	Q353	T439	Q514	W606
P276	C354	V440	F515	N610
F277	T355	F441	Q516	K611
K280	Q359	P443	K519	C612
P281	L362	F444	S520	V613
L282	V365	A445	A521	S614
V283	H366	F446	C522	S615
D284	H367	T447	I523	H616
V285	E368	P448	K524	H619
M289	L369	D449	A525	H620
Y294	Q373	Y451	G526	
T295	Y374	R452	Q527	
P296	F375	W453	Y528	
L297	L376	S454	D529	
F300	Q377	L455	P530	
Q301	Y378	F456	D531	
M302	Q379	R457	N532	
G303	H380	G458	W533	
	Q381	E459	E534	
	P382	K462	L537	
	F383	D538		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.91Å 121.22Å 94.74Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9806	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: 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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/5031	1.05	34/6814 (0.5%)
1	B	0.53	0/5031	1.05	35/6814 (0.5%)
All	All	0.52	0/10062	1.05	69/13628 (0.5%)

There are no bond length outliers.

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	LEU	N-CA-C	-8.97	101.65	114.12
1	B	426	ALA	N-CA-C	-8.78	102.34	113.23
1	B	491	ASP	N-CA-C	8.74	123.24	112.23
1	A	491	ASP	N-CA-C	8.72	123.22	112.23
1	A	426	ALA	N-CA-C	-8.66	102.72	113.28

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	4900	0	4696	233	2
1	B	4900	0	4696	238	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	9806	0	9392	470	2

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 25.

The worst 5 of 470 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:146:ASP:HB3	1:A:147:PRO:HD3	1.39	1.04
1:B:146:ASP:HB3	1:B:147:PRO:HD3	1.39	1.01
1:A:143:LEU:HD22	1:A:148:GLU:HG2	1.42	1.00
1:B:143:LEU:HD22	1:B:148:GLU:HG2	1.46	0.96
1:B:347:ASP:H	1:B:379:GLN:HE22	0.95	0.94

All (2) 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:A:619:HIS:NE2	1:B:134:ASP:OD2[1_554]	2.07	0.13
1:A:134:ASP:OD2	1:B:619:HIS:NE2[1_554]	2.17	0.03

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%)	517 (87%)	58 (10%)	21 (4%)	3	4
1	B	596/607 (98%)	518 (87%)	56 (9%)	22 (4%)	2	3
All	All	1192/1214 (98%)	1035 (87%)	114 (10%)	43 (4%)	2	4

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	147	PRO
1	A	418	LYS
1	A	542	ILE
1	B	24	GLN

5.3.2 Protein sidechains ⓘ

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%)	484 (93%)	38 (7%)	13	29
1	B	522/530 (98%)	485 (93%)	37 (7%)	13	31
All	All	1044/1060 (98%)	969 (93%)	75 (7%)	13	30

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	334	LEU
1	B	537	LEU
1	B	336	CYS
1	B	418	LYS
1	A	378	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	33	ASN
1	B	601	ASN
1	B	311	ASN
1	B	554	ASN
1	B	514	GLN

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 oligosaccharides 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 [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.