Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 10:00 am BST

PDB ID	:	1ICE
Title	:	STRUCTURE AND MECHANISM OF INTERLEUKIN-1BETA CONVERTING ENZYME
Authors	:	Wilson, K.P.; Griffith, J.P.; Kim, E.E.; Navia, M.A.
Deposited on	:	1994-09-29
Resolution	:	2.60 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 (i)) were used in the production of this report:

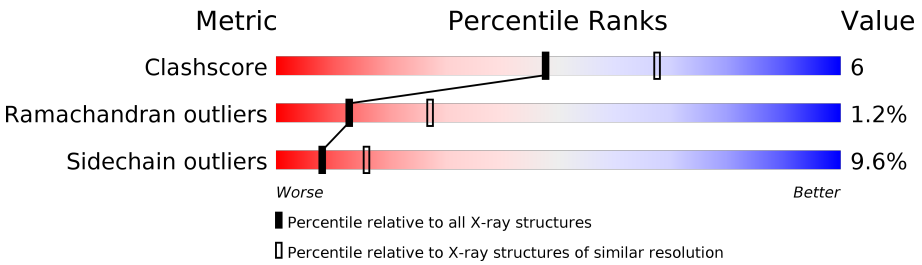
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	167	78% 20% •
2	T	5	80% 20%
3	B	88	69% 25% 5% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2096 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 INTERLEUKIN-1 BETA CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	167	1308	821	228	248	11	6	0	0

- Molecule 2 is a protein called TETRAPEPTIDE ALDEHYDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	T	5	35	23	4	8	0	0	0

- Molecule 3 is a protein called INTERLEUKIN-1 BETA CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	88	719	457	126	129	7	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	13	13	13	0	0
4	B	21	21	21	0	0

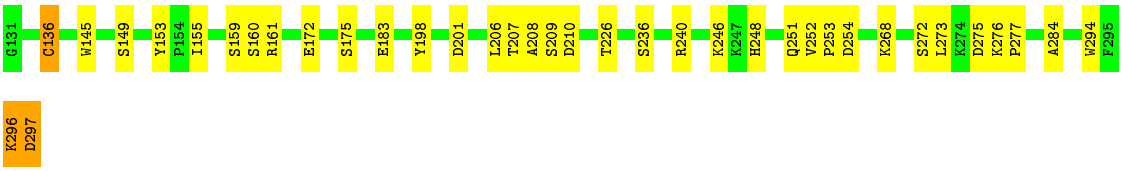
3 Residue-property plots (i)

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: INTERLEUKIN-1 BETA CONVERTING ENZYME

Chain A:



- Molecule 2: TETRAPEPTIDE ALDEHYDE

Chain T:

- Molecule 3: INTERLEUKIN-1 BETA CONVERTING ENZYME

Chain B:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	64.40Å 64.40Å 163.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2096	wwPDB-VP
Average B, all atoms ($Å^2$)	26.0	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: ASA, ACE

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	0.86	2/1330 (0.2%)	1.46	8/1792 (0.4%)
2	T	0.73	0/25	1.47	0/34
3	B	0.93	1/739 (0.1%)	1.62	8/995 (0.8%)
All	All	0.88	3/2094 (0.1%)	1.52	16/2821 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	B	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	TRP	CD2-CE2	8.26	1.51	1.41
3	B	340	TRP	CD2-CE2	7.93	1.50	1.41
1	A	294	TRP	CD2-CE2	6.69	1.49	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145	TRP	CE2-CD2-CG	-12.87	97.00	107.30
3	B	340	TRP	CE2-CD2-CG	-12.79	97.06	107.30
1	A	294	TRP	CE2-CD2-CG	-12.73	97.11	107.30
1	A	145	TRP	CG-CD2-CE3	11.01	143.81	133.90
1	A	294	TRP	CG-CD2-CE3	10.42	143.28	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	294	TRP	CD1-CG-CD2	9.53	113.92	106.30
3	B	340	TRP	CG-CD2-CE3	9.01	142.01	133.90
3	B	340	TRP	CD1-CG-CD2	8.61	113.19	106.30
1	A	145	TRP	CD1-CG-CD2	8.29	112.93	106.30
3	B	371	ARG	NE-CZ-NH1	7.47	124.04	120.30
3	B	371	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	240	ARG	NE-CZ-NH1	6.46	123.53	120.30
3	B	334	THR	N-CA-CB	-6.18	98.56	110.30
3	B	391	ARG	NE-CZ-NH1	5.96	123.28	120.30
3	B	321	ALA	O-C-N	-5.82	113.38	122.70
1	A	161	ARG	NE-CZ-NH2	-5.29	117.66	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	TYR	Sidechain
1	A	296	LYS	Peptide
3	B	360	TYR	Sidechain
3	B	391	ARG	Sidechain

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	1308	0	1315	16	0
2	T	35	0	29	1	0
3	B	719	0	692	13	0
4	A	13	0	0	0	0
4	B	21	0	0	0	1
All	All	2096	0	2036	25	1

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 6.

All (25) 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)
3:B:328:ILE:HG13	3:B:392:VAL:HG22	1.64	0.77
1:A:296:LYS:HG2	1:A:297:ASP:HA	1.66	0.76
1:A:248:HIS:HD2	1:A:254:ASP:H	1.45	0.62
1:A:273:LEU:HD23	1:A:276:LYS:HD2	1.83	0.60
1:A:155:ILE:HG13	3:B:401:PHE:HD2	1.66	0.59
1:A:206:LEU:HB3	1:A:210:ASP:HB2	1.87	0.57
1:A:248:HIS:CD2	1:A:253:PRO:HA	2.40	0.57
1:A:155:ILE:HG13	3:B:401:PHE:CD2	2.40	0.57
1:A:248:HIS:HD2	1:A:253:PRO:HA	1.70	0.56
1:A:236:SER:O	1:A:284:ALA:HA	2.10	0.52
1:A:248:HIS:CD2	1:A:254:ASP:H	2.28	0.51
1:A:207:THR:H	1:A:210:ASP:HB2	1.78	0.49
3:B:380:PRO:HB3	3:B:384:ALA:HB2	1.94	0.48
3:B:334:THR:CG2	3:B:337:ASN:HD22	2.29	0.46
1:A:136:CYS:O	3:B:404:HIS:HE1	1.99	0.46
3:B:401:PHE:O	3:B:402:PRO:C	2.55	0.45
1:A:207:THR:O	1:A:208:ALA:C	2.55	0.45
1:A:153:TYR:CD2	1:A:277:PRO:HG3	2.52	0.45
3:B:334:THR:HG22	3:B:337:ASN:HD22	1.82	0.44
1:A:252:VAL:HA	1:A:253:PRO:HD3	1.74	0.43
2:T:289:ASA:CG	3:B:341:ARG:HH11	2.31	0.43
3:B:341:ARG:HG3	3:B:347:SER:OG	2.18	0.42
1:A:275:ASP:HA	3:B:326:ASP:OD2	2.20	0.42
3:B:325:LYS:HA	3:B:393:THR:HB	2.01	0.41
3:B:352:ARG:HE	3:B:376:SER:HB2	1.85	0.41

All (1) 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)
4:B:285:HOH:O	4:B:288:HOH:O[7_555]	2.08	0.12

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	165/167 (99%)	155 (94%)	9 (6%)	1 (1%)	25 47
2	T	3/5 (60%)	3 (100%)	0	0	100 100
3	B	86/88 (98%)	76 (88%)	8 (9%)	2 (2%)	6 11
All	All	254/260 (98%)	234 (92%)	17 (7%)	3 (1%)	13 27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	343	PRO
1	A	149	SER
3	B	381	ASP

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	147/149 (99%)	133 (90%)	14 (10%)	8 16
2	T	2/2 (100%)	2 (100%)	0	100 100
3	B	79/79 (100%)	71 (90%)	8 (10%)	7 14
All	All	228/230 (99%)	206 (90%)	22 (10%)	8 16

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	CYS
1	A	159	SER
1	A	160	SER
1	A	172	GLU
1	A	175	SER
1	A	183	GLU
1	A	201	ASP
1	A	209	SER

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Mol	Chain	Res	Type
1	A	226	THR
1	A	246	LYS
1	A	251	GLN
1	A	268	LYS
1	A	272	SER
1	A	297	ASP
3	B	333	SER
3	B	334	THR
3	B	339	SER
3	B	343	PRO
3	B	344	THR
3	B	352	ARG
3	B	363	SER
3	B	393	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	HIS
3	B	322	HIS
3	B	337	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ASA	T	289	1,2	3,7,7	3.56	1 (33%)	1,8,8	0.64	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	ASA	T	289	1,2	-	2/3/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	289	ASA	O-C	6.14	1.44	1.19

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	289	ASA	N-CA-CB-CG
2	T	289	ASA	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	289	ASA	1	0

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 (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.