

wwPDB X-ray Structure Validation Summary Report (i)

Aug 2, 2023 – 02:04 AM EDT

PDB ID : 1B0J

Title : CRYSTAL STRUCTURE OF ACONITASE WITH ISOCITRATE

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Deposited on : 1998-11-10

Resolution : 2.50 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)

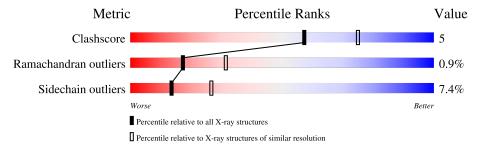
Validation Pipeline (wwPDB-VP) : 2.34

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 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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	754	78%	18%	



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6153 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.

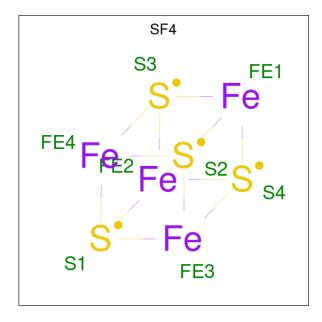
• Molecule 1 is a protein called ACONITATE HYDRATASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	753	Total 5814	C 3666	N 1034	O 1092	S 22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

	Chain	Residue	Modelled	Actual	Comment	Reference
	A	642	ALA	SER	engineered mutation	UNP P16276
Ī	A	648	ALA	ARG	conflict	UNP P16276

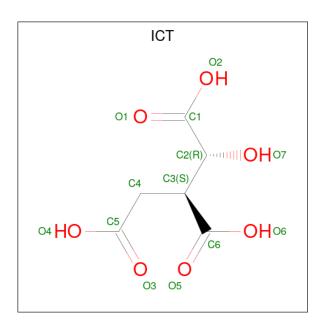
• Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
9	Λ	1	Total	Fe	S	0	0
2	Λ	1	8	4	4	0	0

• Molecule 3 is ISOCITRIC ACID (three-letter code: ICT) (formula: $C_6H_8O_7$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 13	C 6	O 7	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	318	Total O 318 318	0	0

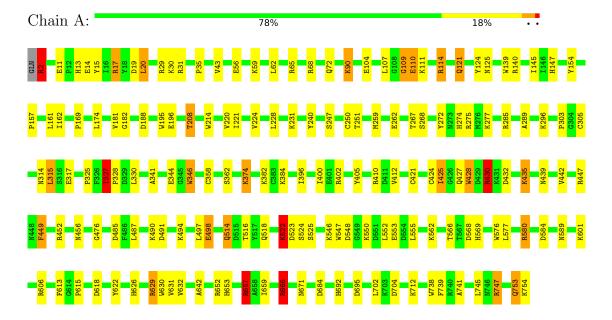


3 Residue-property plots (i)

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: ACONITATE HYDRATASE





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants	187.40Å 72.10Å 73.90Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 77.70°	Depositor
Resolution (Å)	20.00 - 2.50	Depositor
% Data completeness	88.1 (20.00-2.50)	Depositor
(in resolution range)	00.1 (20.00 2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6153	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: SF4, ICT

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.88	0/5941	1.62	89/8049 (1.1%)	

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	1

There are no bond length outliers.

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	A	580	ARG	NE-CZ-NH1	22.36	131.48	120.30
1	A	430	ARG	NE-CZ-NH2	-19.18	110.71	120.30
1	A	447	ARG	NE-CZ-NH2	-14.16	113.22	120.30
1	A	580	ARG	NE-CZ-NH2	-13.39	113.61	120.30
1	A	325	PRO	CA-C-N	10.44	140.17	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Group
1	A	666	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	5814	0	5804	57	0
2	A	8	0	0	1	0
3	A	13	0	5	2	0
4	A	318	0	0	6	0
All	All	6153	0	5809	57	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 5.

The worst 5 of 57 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:430:ARG:HH22	1:A:439:ASN:HD21	1.30	0.79
1:A:430:ARG:HD2	1:A:432:ASP:OD1	1.96	0.66
1:A:566:THR:HG22	1:A:568:ASP:H	1.61	0.64
1:A:629:ARG:HG2	1:A:657:ARG:HD3	1.80	0.64
1:A:449:PHE:CD2	1:A:566:THR:HG21	2.36	0.60

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	751/754 (100%)	703 (94%)	41 (6%)	7 (1%)		17	31

5 of 7 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	524	SER
1	A	753	GLN
1	A	109	GLY
1	A	296	LYS
1	A	523	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	621/622 (100%)	575 (93%)	46 (7%)	13 27		

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	514	GLN
1	A	601	LYS
1	A	516	THR
1	A	553	GLU
1	A	631	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	519	HIS
1	A	653	HIS
1	A	536	GLN
1	A	671	ASN
1	A	626	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)

2 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	Во	ond leng	$ ag{ths}$	В	ond ang	les
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	A	755	1,3,4	0,12,12	-	-	=		
3	ICT	A	756	2	12,12,12	1.21	0	13,16,16	1.21	2 (15%)

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	SF4	A	755	1,3,4	-	-	0/6/5/5
3	ICT	A	756	2	-	7/16/16/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
3	A	756	ICT	C3-C4-C5	-2.38	109.30	114.04
3	A	756	ICT	O7-C2-C1	-2.34	105.77	110.66

There are no chirality outliers.



5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	756	ICT	C6-C3-C4-C5
3	A	756	ICT	C2-C3-C4-C5
3	A	756	ICT	C4-C3-C6-O5
3	A	756	ICT	C4-C3-C6-O6
3	A	756	ICT	O7-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	755	SF4	1	0
3	A	756	ICT	2	0

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.

