

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1C97
Title	:	S642A:ISOCITRATE COMPLEX OF ACONITASE
Authors	:	Lloyd, S.J.; Lauble, H.; Prasad, G.S.; Stout, C.D.
Deposited on		
Resolution	:	1.98 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 (1)) were used in the production of this report:

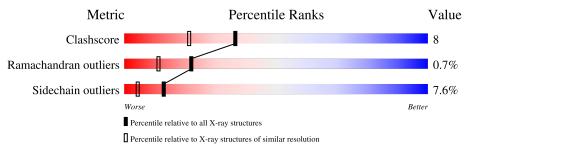
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

The reported resolution of this entry is 1.98 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)

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	А	753	73%	23%	•••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	А	755	-	-	Х	-
4	ICT	А	756	-	Х	-	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6429 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 MITOCHONDRIAL ACONITASE.

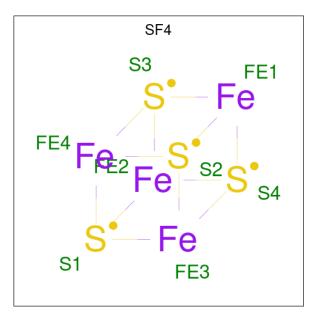
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	753	Total 5814	C 3666	N 1034	O 1092	S 22	0	0	0

Chain Residue Modelled Actual Comment Reference HIS UNP P20004 А 13 ASN conflict ASP ASN А 26conflict UNP P20004 Α 303 PRO conflict UNP P20004 SER А 310 VAL LEU conflict UNP P20004 А 382LYS GLN conflict UNP P20004 А VAL ILE conflict UNP P20004 408UNP P20004 А 528ARG GLU conflict А 550LYS ARG conflict UNP P20004 <u>UNP</u> P20004 ILE VAL А 597 conflict А ARG UNP P20004 600 GLY conflict А 625GLN LYS conflict UNP P20004 А 642 ALA SER UNP P20004 engineered mutation А 647 SER ALA conflict UNP P20004 Α GLN LYS UNP P20004 700 conflict LYS А 712THRconflict UNP P20004 А 753 GLN LYS UNP P20004 conflict

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



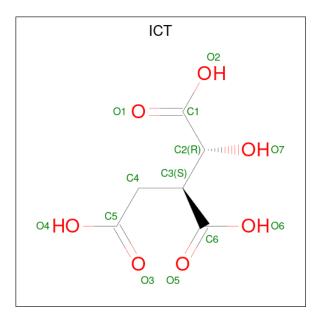


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	А	1	Total 8	Fe 4	${S \atop 4}$	0	0

• Molecule 3 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total O 1 1	0	0

• Molecule 4 is ISOCITRIC ACID (three-letter code: ICT) (formula: $C_6H_8O_7$).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	А	1	Total 13	C 6	O 7	0	0

• Molecule 5 is water.

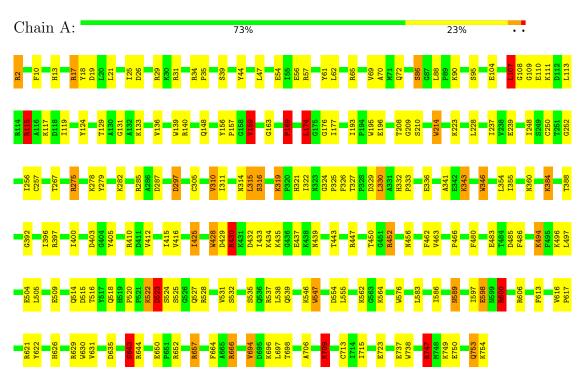
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	593	Total O 593 593	0	0



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: MITOCHONDRIAL ACONITASE



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	176.40Å 71.40Å 71.90Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 - 1.98	Depositor
% Data completeness	(Not available) (20.00-1.98)	Depositor
(in resolution range)	(1100 available) (20.00 1.50)	Depositor
R_{merge}	0.11	Depositor
R _{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.218 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6429	wwPDB-VP
Average B, all atoms $(Å^2)$	24.0	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: O, ICT, SF4

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).

Mal	Chain	Bo	nd lengths	Bond angles		
Mol Chain		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.01	5/5941~(0.1%)	1.68	99/8049~(1.2%)	

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	А	531	VAL	CA-CB	5.72	1.66	1.54
1	А	239	GLU	CB-CG	-5.63	1.41	1.52
1	А	310	VAL	CA-CB	5.49	1.66	1.54
1	А	316	SER	CB-OG	-5.40	1.35	1.42
1	А	195	TRP	CD1-NE1	-5.24	1.29	1.38

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	666	ARG	NE-CZ-NH1	-27.59	106.50	120.30
1	А	666	ARG	NE-CZ-NH2	25.67	133.13	120.30
1	А	57	ARG	NE-CZ-NH2	12.17	126.39	120.30
1	А	195	TRP	CD1-CG-CD2	10.84	114.97	106.30
1	А	410	ARG	NE-CZ-NH1	-10.63	114.98	120.30

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	5814	0	5803	91	0
2	А	8	0	0	2	0
3	А	1	0	0	0	0
4	А	13	0	4	3	0
5	А	593	0	0	4	0
All	All	6429	0	5807	91	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 8.

The worst 5 of 91 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:643:SER:HB2	4:A:756:ICT:O6	1.71	0.90
1:A:504:GLU:HG2	1:A:505:LEU:HG	1.58	0.85
1:A:433:ILE:HD12	1:A:456:ASN:HD22	1.47	0.78
1:A:520:PRO:HB2	1:A:522:LYS:HG2	1.68	0.74
1:A:113:LEU:HG	1:A:117:LYS:HE2	1.71	0.71

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	Analysed Favoured Allowed		Outliers	Percentiles	
1	А	751/753~(100%)	712 (95%)	34~(4%)	5(1%)	22 11	

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	450	THR
1	А	452	ARG
1	А	169	PRO

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Mol	Chain	Res	Type
1	А	525	SER
1	А	109	GLY

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	621/621~(100%)	574 (92%)	47 (8%)	13 4		

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	452	ARG
1	А	528	ARG
1	А	494	LYS
1	А	515	ASP
1	А	589	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	А	519	HIS
1	А	536	GLN
1	А	671	ASN
1	А	589	ASN
1	А	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)

Of 3 ligands modelled in this entry, 1 is 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).

Mal	Turne	Chain	Dec	Link	Bo	ond leng	\mathbf{ths}	B	ond ang	les
INIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	SF4	А	755	3,1,4	0,12,12	-	-	-		
4	ICT	А	756	3,2	12,12,12	1.95	5 (41%)	13,16,16	<mark>3.59</mark>	6 (46%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	756	ICT	O7-C2	3.30	1.48	1.42
4	А	756	ICT	C2-C1	-3.10	1.48	1.52
4	А	756	ICT	C3-C6	-2.77	1.46	1.51
4	А	756	ICT	O6-C6	-2.20	1.23	1.30
4	А	756	ICT	O1-C1	2.09	1.28	1.22

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
4	А	756	ICT	O6-C6-C3	6.82	132.81	114.03
4	А	756	ICT	O7-C2-C1	-5.71	98.69	110.66

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	756	ICT	O7-C2-C3	5.45	123.82	110.58
4	А	756	ICT	C3-C4-C5	-4.62	104.84	114.04
4	А	756	ICT	O5-C6-C3	-4.37	112.01	122.95

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There are no chirality outliers.

5 of 7 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	755	SF4	2	0
4	А	756	ICT	3	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.

