wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 09:32 AM EST

PDB ID	:	1C96
Title	:	S642A:CITRATE COMPLEX OF ACONITASE
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Deposited on	:	1999-07-31
Resolution	:	1.81 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:

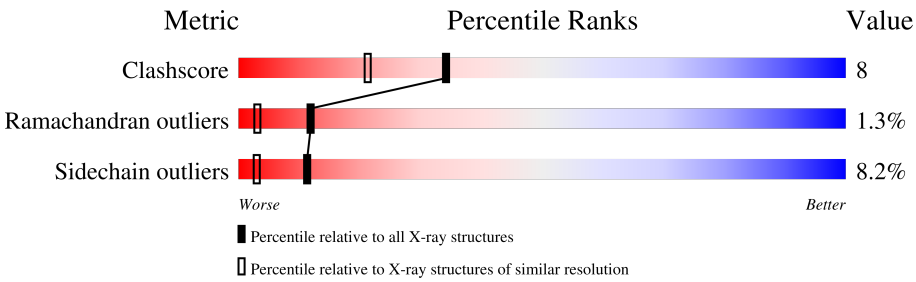
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

The reported resolution of this entry is 1.81 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	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)

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	753	71% 23% 5% •

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
3	SF4	A	755	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6510 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.

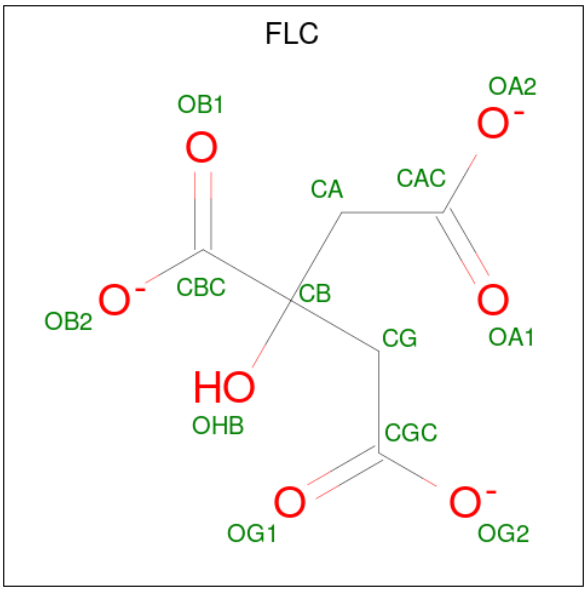
- Molecule 1 is a protein called MITOCHONDRIAL ACONITASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	753	5811	3665	1034	1090	22	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

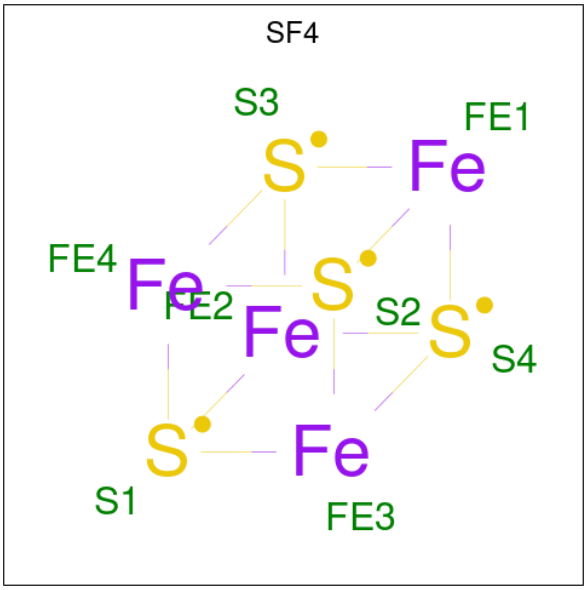
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	HIS	ASN	conflict	UNP P20004
A	26	ASP	ASN	conflict	UNP P20004
A	303	PRO	SER	conflict	UNP P20004
A	310	VAL	LEU	conflict	UNP P20004
A	382	LYS	GLN	conflict	UNP P20004
A	408	VAL	ILE	conflict	UNP P20004
A	528	ARG	GLU	conflict	UNP P20004
A	530	ALA	ASP	conflict	UNP P20004
A	550	LYS	ARG	conflict	UNP P20004
A	597	ILE	VAL	conflict	UNP P20004
A	600	ARG	GLY	conflict	UNP P20004
A	625	GLN	LYS	conflict	UNP P20004
A	642	ALA	SER	engineered mutation	UNP P20004
A	647	SER	ALA	conflict	UNP P20004
A	700	GLN	LYS	conflict	UNP P20004
A	712	LYS	THR	conflict	UNP P20004
A	753	GLN	LYS	conflict	UNP P20004

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



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

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0

- Molecule 4 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	677	677	677	0	0

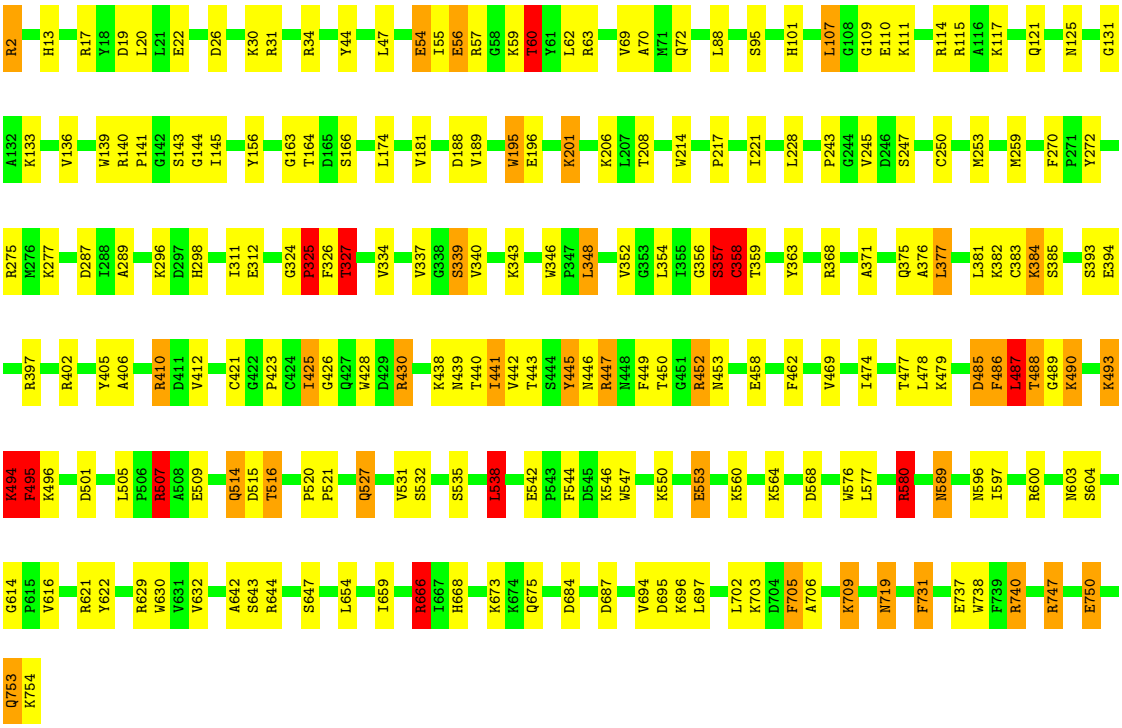
3 Residue-property plots (i)

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

Chain A: 71% 23% 5% •



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 a, b, c, α, β, γ	176.10Å 71.40Å 71.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.81	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.81)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.225 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6510	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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, FLC, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.01	5/5938 (0.1%)	1.69	103/8045 (1.3%)

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	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	643	SER	N-CA	-8.97	1.28	1.46
1	A	195	TRP	CD1-NE1	-5.26	1.29	1.38
1	A	195	TRP	CG-CD2	-5.08	1.35	1.43
1	A	201	LYS	CD-CE	5.06	1.64	1.51
1	A	114	ARG	NE-CZ	5.02	1.39	1.33

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	666	ARG	NE-CZ-NH2	18.74	129.67	120.30
1	A	666	ARG	NE-CZ-NH1	-15.68	112.46	120.30
1	A	402	ARG	NE-CZ-NH1	-13.56	113.52	120.30
1	A	114	ARG	NE-CZ-NH2	12.58	126.59	120.30
1	A	195	TRP	CD1-CG-CD2	10.87	114.99	106.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	GLY	Peptide
1	A	580	ARG	Sidechain
1	A	622	TYR	Sidechain
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	5811	0	5805	98	0
2	A	13	0	5	3	0
3	A	8	0	0	3	0
4	A	1	0	0	0	0
5	A	677	0	0	8	0
All	All	6510	0	5810	98	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 98 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:632:VAL:HB	1:A:659:ILE:HG23	1.70	0.72
1:A:145:ILE:HG21	1:A:358:CYS:HB2	1.74	0.69
1:A:737:GLU:HG2	1:A:740:ARG:HH11	1.61	0.65
1:A:358:CYS:HB3	3:A:755:SF4:S4	2.37	0.64
1:A:430:ARG:HH22	1:A:439:ASN:HD21	1.46	0.64

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	751/753 (100%)	706 (94%)	35 (5%)	10 (1%)	12 3

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	SER
1	A	495	PHE
1	A	485	ASP
1	A	109	GLY
1	A	494	LYS

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	620/620 (100%)	569 (92%)	51 (8%)	11 3

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	490	LYS
1	A	527	GLN
1	A	747	ARG
1	A	494	LYS
1	A	507	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	671	ASN
1	A	753	GLN
1	A	719	ASN
1	A	527	GLN

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Mol	Chain	Res	Type
1	A	653	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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SF4	A	755	2,1,4	0,12,12	-	-	-		
2	FLC	A	756	3	12,12,12	4.12	5 (41%)	17,17,17	2.08	6 (35%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	756	FLC	CB-CBC	11.10	1.64	1.53
2	A	756	FLC	CA-CB	5.59	1.60	1.53
2	A	756	FLC	CG-CB	4.96	1.60	1.53
2	A	756	FLC	OA1-CAC	3.03	1.32	1.22
2	A	756	FLC	OG2-CGC	-2.35	1.22	1.30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	756	FLC	CB-CA-CAC	4.62	125.00	113.81
2	A	756	FLC	OB2-CBC-CB	3.83	119.70	113.05
2	A	756	FLC	OHB-CB-CBC	3.30	113.50	108.86
2	A	756	FLC	CB-CG-CGC	2.29	119.36	113.81
2	A	756	FLC	CG-CB-CA	-2.28	103.21	109.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	756	FLC	CA-CB-CG-CGC
2	A	756	FLC	CBC-CB-CG-CGC
2	A	756	FLC	OHB-CB-CG-CGC

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	755	SF4	3	0
2	A	756	FLC	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.