



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2017 – 12:37 AM EST

PDB ID : 1CSR
Title : Alpha-fluoro acid and alpha-fluoro amide analogs of acetyl-coa as inhibitors of
of citrate synthase: effect of pka matching on binding affinity and hydrogen
bond length
Authors : Usher, K.C.; Remington, S.J.
Deposited on : unknown
Resolution : 1.70 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

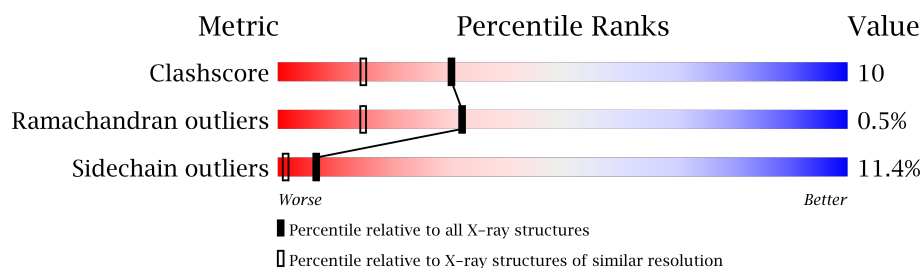
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	435	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3597 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.

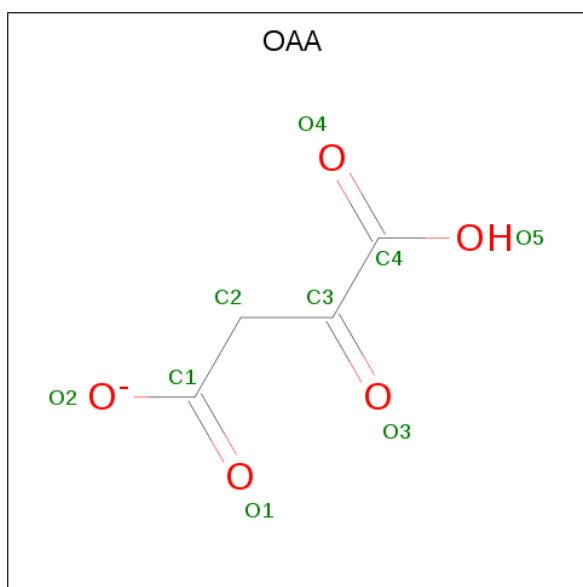
- Molecule 1 is a protein called CITRATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3391	2167	583	625	16			

There are 25 discrepancies between the modelled and reference sequences:

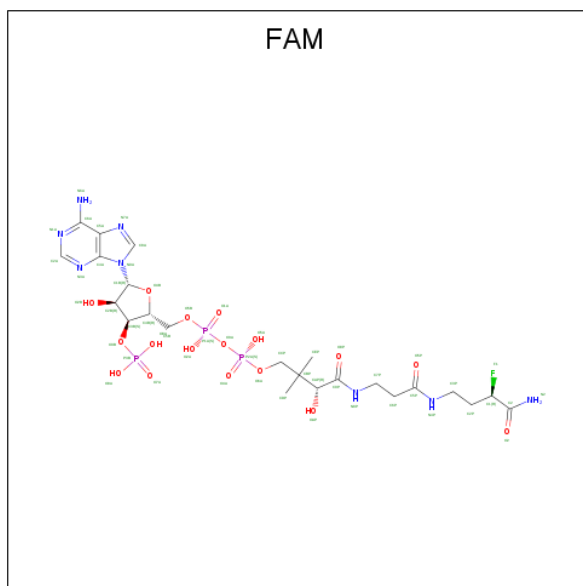
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	VAL	ILE	CONFLICT	UNP P23007
A	12	SER	ASP	CONFLICT	UNP P23007
A	32	ALA	VAL	CONFLICT	UNP P23007
A	41	SER	MET	CONFLICT	UNP P23007
A	52	ILE	VAL	CONFLICT	UNP P23007
A	69	PHE	TYR	CONFLICT	UNP P23007
A	77	LEU	MET	CONFLICT	UNP P23007
A	82	GLY	LYS	CONFLICT	UNP P23007
A	104	PRO	GLU	CONFLICT	UNP P23007
A	110	VAL	LEU	CONFLICT	UNP P23007
A	163	ASN	HIS	CONFLICT	UNP P23007
A	170	PHE	LEU	CONFLICT	UNP P23007
A	171	VAL	ILE	CONFLICT	UNP P23007
A	175	ALA	CYS	CONFLICT	UNP P23007
A	196	ALA	GLU	CONFLICT	UNP P23007
A	222	PRO	ALA	CONFLICT	UNP P23007
A	283	LEU	VAL	CONFLICT	UNP P23007
A	286	SER	THR	CONFLICT	UNP P23007
A	291	ASP	GLU	CONFLICT	UNP P23007
A	292	LEU	VAL	CONFLICT	UNP P23007
A	294	ALA	LYS	CONFLICT	UNP P23007
A	296	ALA	VAL	CONFLICT	UNP P23007
A	343	SER	HIS	CONFLICT	UNP P23007
A	428	ALA	ASP	CONFLICT	UNP P23007
A	431	GLU	ILE	CONFLICT	UNP P23007

- Molecule 2 is OXALOACETATE ION (three-letter code: OAA) (formula: C₄H₃O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is ALPHA-FLUORO-AMIDOCARBOXYMETHYLDETHIA COENZYME A COMPLEX (three-letter code: FAM) (formula: $C_{23}H_{38}FN_8O_{17}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	P	0	0
			52	23	1	8	17	3		

- Molecule 4 is water.

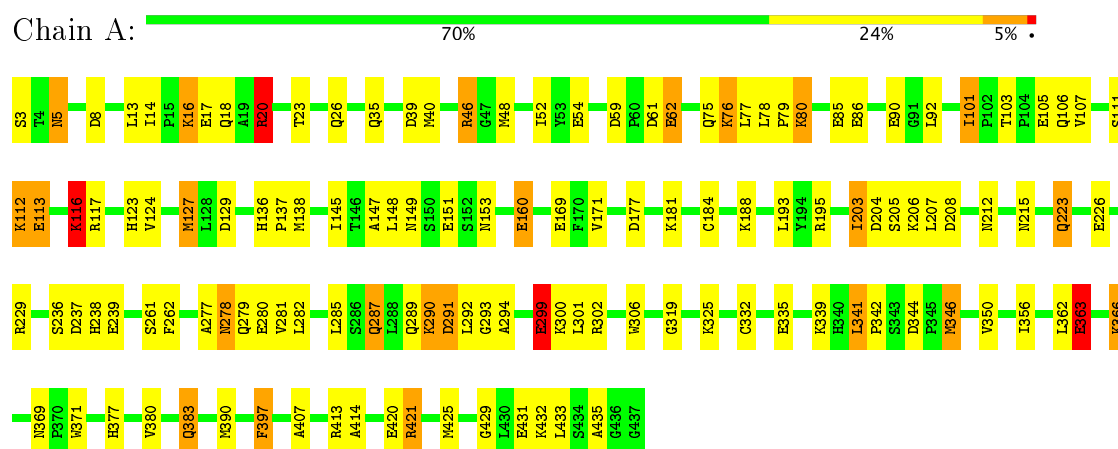
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	145	Total 145	O 145	0	0

3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: CITRATE SYNTHASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.39 Å 78.43 Å 58.47 Å 90.00° 78.86° 90.00°	Depositor
Resolution (Å)	25.00 – 1.70	Depositor
% Data completeness (in resolution range)	75.0 (25.00-1.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3597	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: OAA, FAM

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	0.93	20/3476 (0.6%)	1.36	25/4721 (0.5%)

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

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	GLU	CD-OE1	7.22	1.33	1.25
1	A	105	GLU	CD-OE1	7.19	1.33	1.25
1	A	299	GLU	CD-OE2	7.01	1.33	1.25
1	A	363	GLU	CD-OE2	7.00	1.33	1.25
1	A	54	GLU	CD-OE1	6.93	1.33	1.25

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ASP	CB-CG-OD2	-9.87	109.42	118.30
1	A	344	ASP	CB-CG-OD1	-8.70	110.47	118.30
1	A	39	ASP	CB-CG-OD1	7.68	125.21	118.30
1	A	20	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	8	ASP	CB-CG-OD1	-6.75	112.23	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	287	GLN	Sidechain

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	3391	0	3370	72	1
2	A	9	0	2	0	0
3	A	52	0	34	1	0
4	A	145	0	0	4	1
All	All	3597	0	3406	72	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 10.

The worst 5 of 72 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:20:ARG:O	4:A:664:HOH:O	1.77	1.01
1:A:78:LEU:O	1:A:80:LYS:NZ	2.09	0.84
1:A:136:HIS:HD2	1:A:138:MET:H	1.26	0.82
1:A:113:GLU:HA	1:A:116:LYS:HZ3	1.49	0.77
1:A:306:TRP:HZ2	1:A:363:GLU:HG2	1.50	0.76

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)
4:A:566:HOH:O	4:A:566:HOH:O[2_555]	1.32	0.88
1:A:35:GLN:NE2	1:A:35:GLN:NE2[2_555]	2.01	0.19

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	433/435 (100%)	418 (96%)	13 (3%)	2 (0%)	32 15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	ALA
1	A	435	ALA

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	361/361 (100%)	320 (89%)	41 (11%)	7 1

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	SER
1	A	278	ASN
1	A	397	PHE
1	A	223	GLN
1	A	238	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	211	HIS
1	A	278	ASN
1	A	153	ASN
1	A	289	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 carbohydrates 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	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	FAM	A	700	-	45,54,54	0.76	1 (2%)	49,81,81	1.22	4 (8%)
2	OAA	A	702	-	2,8,8	0.88	0	2,10,10	0.93	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
3	FAM	A	700	-	-	0/49/70/70	0/3/3/3
2	OAA	A	702	-	-	0/2/8/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	FAM	C6P-C5P	2.12	1.55	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	FAM	C7P-C6P-C5P	2.51	116.26	112.22
3	A	700	FAM	O8A-P3B-O7A	2.60	120.67	110.50
3	A	700	FAM	C1B-N9A-C4A	3.17	132.11	126.64
3	A	700	FAM	OAP-CAP-CBP	4.18	120.08	110.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	FAM	1	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 ⓘ

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.