



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 16, 2018 – 08:51 pm GMT

PDB ID : 5CSC  
Title : STRUCTURE OF AN OPEN FORM OF CHICKEN HEART CITRATE  
SYNTHASE AT 2.8 ANGSTROMS RESOLUTION  
Authors : Liao, D.-I.; Karpusas, M.; Remington, S.J.  
Deposited on : 1990-05-07  
Resolution : 2.80 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](mailto: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 ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

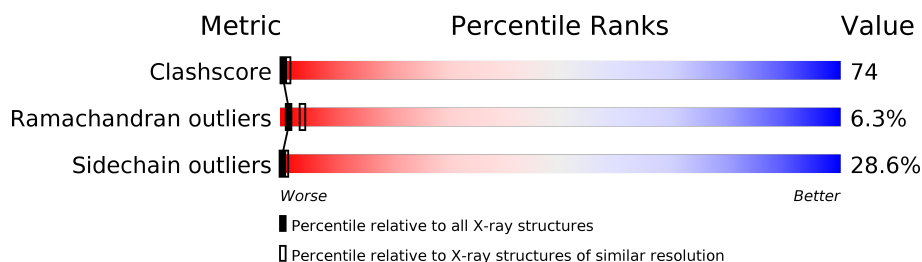
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	122078	3207 (2.80-2.80)
Ramachandran outliers	120005	3156 (2.80-2.80)
Sidechain outliers	119972	3158 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	433	
2	B	429	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6606 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	429	Total	C	N	O	S	0	0	0
			3303	2112	571	603	17			

- Molecule 2 is a protein called CITRATE SYNTHASE.

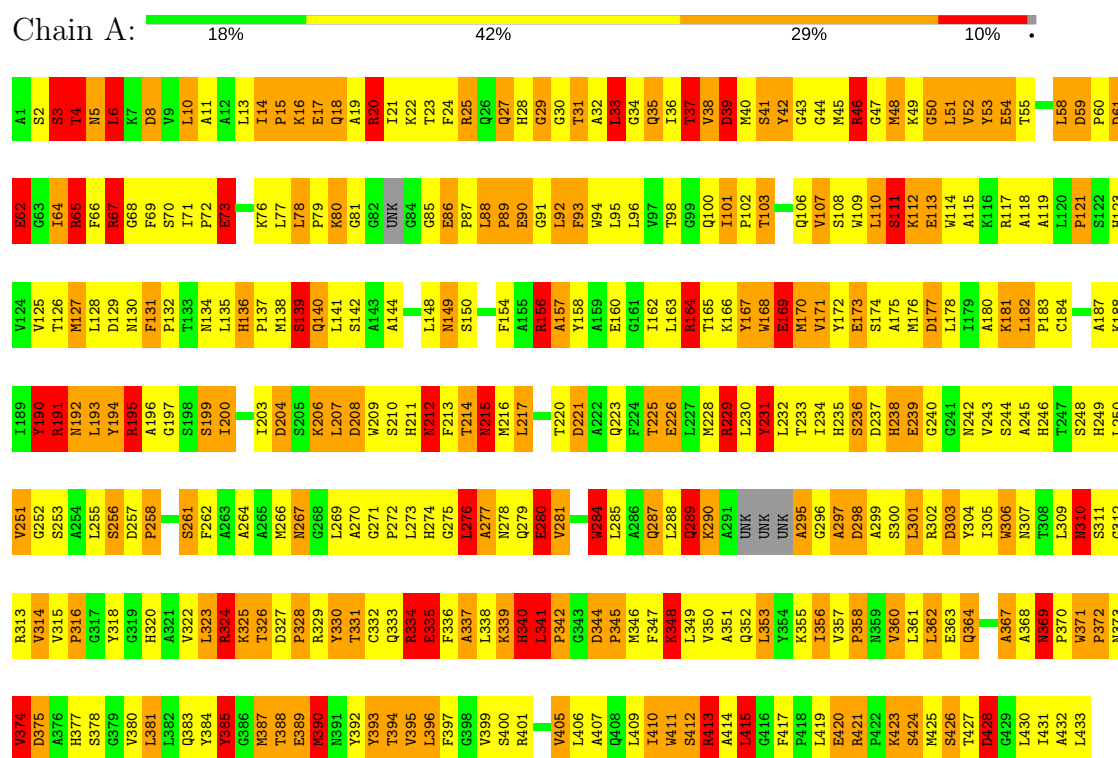
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	429	Total	C	N	O	S	0	0	0
			3303	2112	571	603	17			

### 3 Residue-property plots

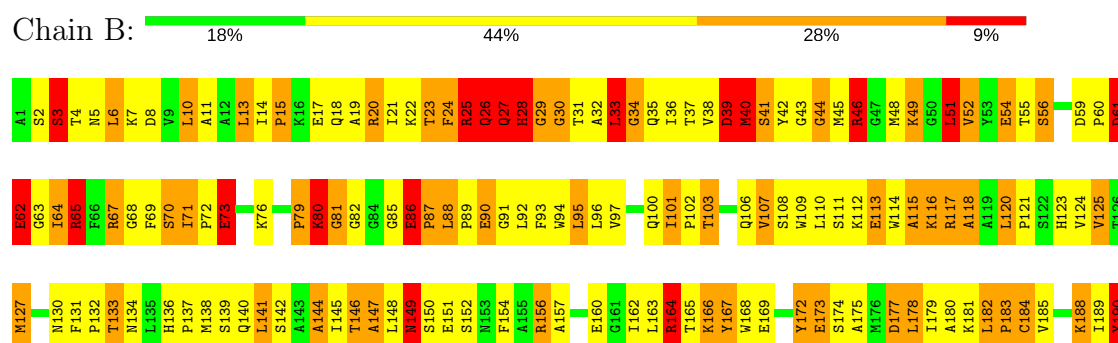
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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



#### • Molecule 2: CITRATE SYNTHASE



G379	V380	L381	L382	Q383	Y384	Y385	G386	M387	T388	E389	M390	N391	Y392	Y393	T394	V395	L396	F397		S400	R401	A402	L403	G404	V405	L406	A407	Q408	L409	I410	W411	S412	R413	A414	L415	G416	F417		E420	R421	P422	K423	S424	M425	S426	T427	D428	G429	L430	I431	A432	L433							
L255	S256	D257	P258	Y259	L260	S261	F262	A263	A264	A265	M266	M267	G268	L269	A270	G271	P272	L273	H274	G275	L276	A277	N278	Q279	E280	V281	L282	G283	W284	L285	A286	Q287	L288	Q289	K290	A291	A295	G296	D298	A299	S300	L301	R302	D303	Y304	I305	M306	N307	T308	L309	N310	S311	G312	R313	V314	V315	P316	V251	G317
Y318	G319	H320	A321	V322	L323	R324	K325	T326	D327	P328	R329	Y330	T331	G332	Q333	R334	E335	F336	A337	L338	K339	H340	L341	P342	G343	D344	P345	M346	F347	K348	L349	V350	A351	Q352	L353	Y354	K355	L356	V357	P358	N359	V360	L361	L362	E363	Q364		A367	A368	N369	P370	N371	P372	N373	V374	D375	A376	H377	S378
R191	N192	L193	Y194	R195	A196	G197	S198	S199	L200	G201	A202	L203	D204	S205	K206	L207	D208	W209	S210	H211	N212	F213	T214	N215	W216	L217		T220	D221	A222	Q223	F224	T225	E226	K227	W228	R229	L230	Y231	L232	T233	L234	H235	S236	D237	H238	E239		N242	V243	S244	A245	H246	T247	S248	H249	L250	V251	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.85Å 58.85Å 259.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	1.84	51/3383 (1.5%)	2.05	103/4594 (2.2%)
2	B	1.92	67/3383 (2.0%)	2.06	96/4594 (2.1%)
All	All	1.88	118/6766 (1.7%)	2.05	199/9188 (2.2%)

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	7	5
2	B	5	3
All	All	12	8

The worst 5 of 118 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	363	GLU	CD-OE2	13.68	1.40	1.25
1	A	239	GLU	CD-OE2	10.55	1.37	1.25
2	B	173	GLU	CD-OE2	9.92	1.36	1.25
1	A	226	GLU	CD-OE2	9.82	1.36	1.25
1	A	73	GLU	CD-OE2	9.64	1.36	1.25

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	117	ARG	NE-CZ-NH1	16.55	128.57	120.30
1	A	334	ARG	NE-CZ-NH1	15.57	128.09	120.30
2	B	421	ARG	NE-CZ-NH1	14.51	127.55	120.30
2	B	413	ARG	NE-CZ-NH1	13.73	127.17	120.30
2	B	413	ARG	NE-CZ-NH2	-13.56	113.52	120.30

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	4	THR	CA
1	A	5	ASN	CA
1	A	51	LEU	CA
1	A	289	GLN	CA
1	A	340	HIS	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	ASN	Sidechain
1	A	337	ALA	Mainchain
1	A	339	LYS	Mainchain
1	A	348	LYS	Mainchain
1	A	385	TYR	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	3303	0	3288	489	26
2	B	3303	0	3288	535	26
All	All	6606	0	6576	972	26

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 74.

The worst 5 of 972 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:46:ARG:NH1	1:A:46:ARG:HB2	1.52	1.22
1:A:33:LEU:HD11	2:B:433:LEU:HD21	1.16	1.13
2:B:86:GLU:HG3	2:B:230:LEU:HB2	1.31	1.12
2:B:79:PRO:HG2	2:B:107:VAL:HG21	1.33	1.11
2:B:341:LEU:HD22	2:B:384:TYR:CD2	1.85	1.10

The worst 5 of 26 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)
1:A:220:THR:CB	2:B:290:LYS:O[3_664]	1.26	0.94
1:A:195:ARG:NH2	2:B:300:SER:OG[3_664]	1.27	0.93
1:A:195:ARG:CZ	2:B:300:SER:OG[3_664]	1.47	0.73
1:A:195:ARG:CD	2:B:297:ALA:CB[3_664]	1.48	0.72
1:A:290:LYS:CA	2:B:220:THR:OG1[3_764]	1.49	0.71

## 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	423/433 (98%)	319 (75%)	77 (18%)	27 (6%)	1	4
2	B	423/429 (99%)	325 (77%)	72 (17%)	26 (6%)	1	4
All	All	846/862 (98%)	644 (76%)	149 (18%)	53 (6%)	1	4

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	14	ILE
1	A	67	ARG
1	A	164	ARG
2	B	3	SER

### 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	344/345 (100%)	240 (70%)	104 (30%)	0	1
2	B	344/345 (100%)	251 (73%)	93 (27%)	0	1
All	All	688/690 (100%)	491 (71%)	197 (29%)	0	1

5 of 197 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	LEU
2	B	26	GLN
2	B	383	GLN
1	A	387	MET
1	A	415	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	383	GLN
2	B	28	HIS
2	B	352	GLN
2	B	26	GLN
2	B	100	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	291:ALA	C	295:ALA	N	9.25
1	B	82:GLY	C	84:GLY	N	3.42

## 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.