wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:32 PM GMT

PDB ID	:	5CSC
Title	:	STRUCTURE OF AN OPEN FORM OF CHICKEN HEART CITRATE SYNTHASE AT 2.8 ANGSTROMS RESOLUTION
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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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

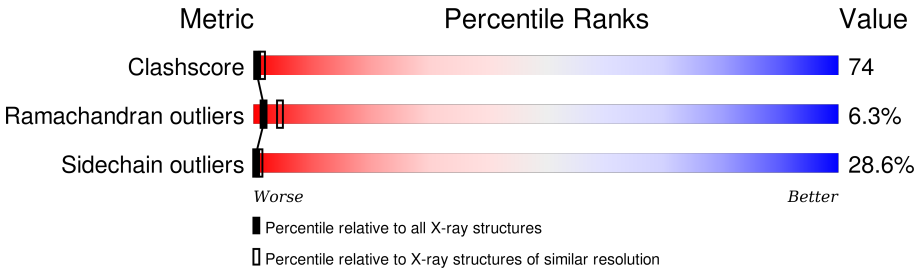
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 >=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 <=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	18% 42% 29% 10%
2	B	429	18% 44% 28% 9%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	429	3303	2112	571	603	17	0	0	0

- Molecule 2 is a protein called CITRATE SYNTHASE.

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

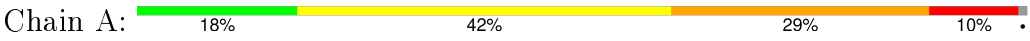
3 Residue-property plots (i)

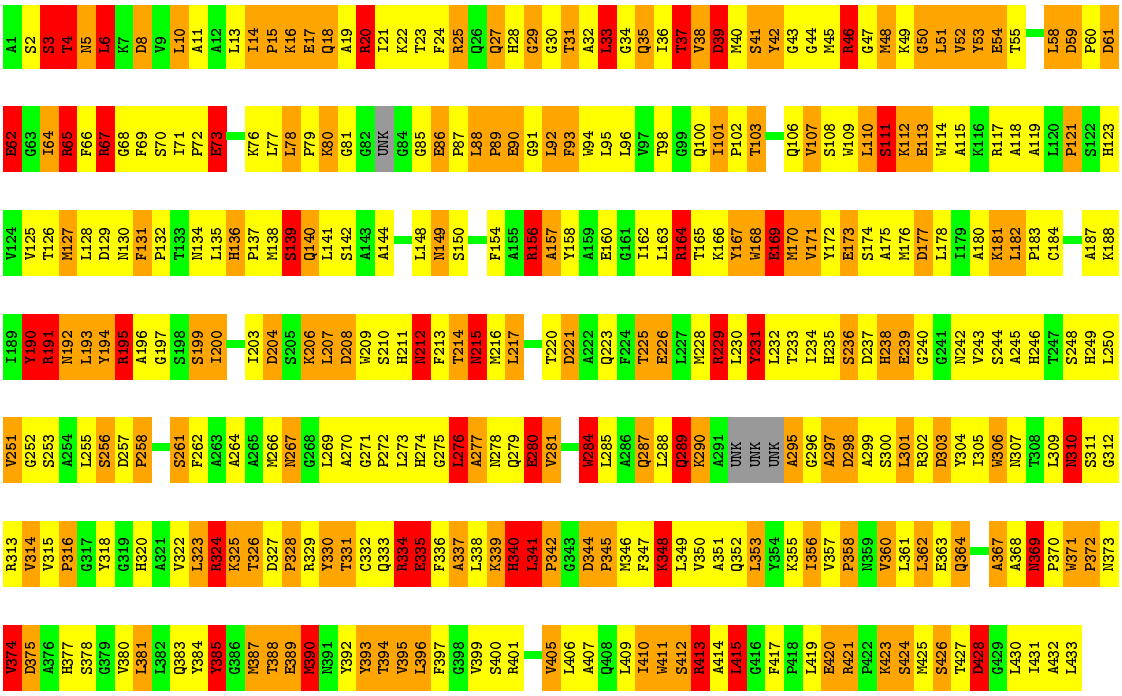
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

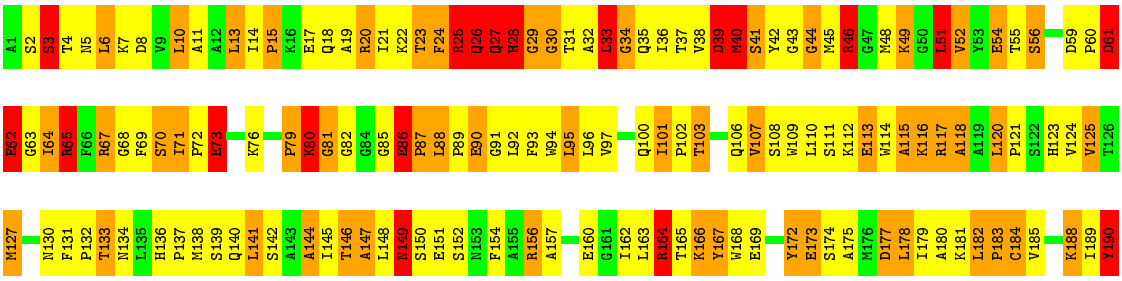
Chain A:

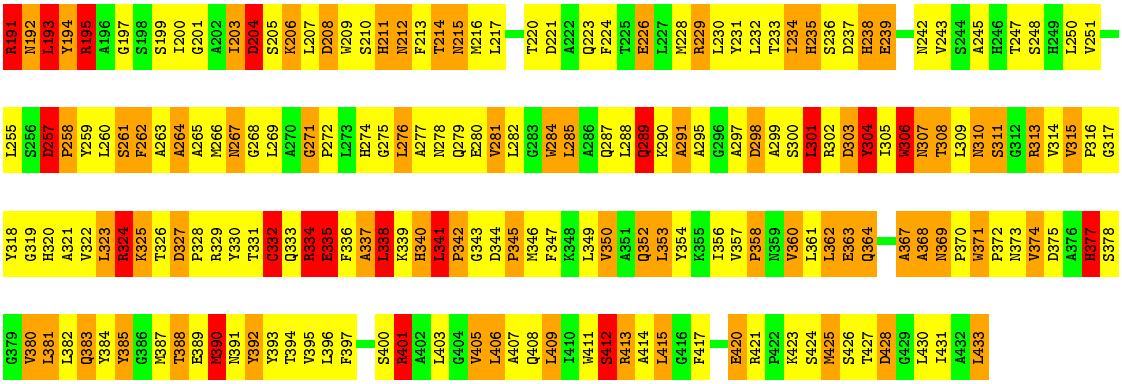




- Molecule 2: CITRATE SYNTHASE

Chain B:




R191 N192 L193 Y194 R195 A196 G197 S198 S199 I200 G201 A202 I203 D204 S205 K206 L207 D208 W209 S210 H211 N212 F213 T214 N215 M216 L217 T220 D221 A222 Q223 F224 T225 E226 L227 M228 R229 L230 Y231 L232 T233 I234 H235 S236 D237 H238 E239 N242 V243 S244 A245 H246 T247 S248 H249 L250 V251
L255 S256 D257 P258 Y259 L260 S261 F262 A263 A264 A265 M266 N267 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 A297 D298 A299 S300 L301 R302 D303 Y304 I305 W306 N307 T308 L309 N310 S311 G312 R313 V314 V315 P316 G317
Y318 G319 H320 A321 V322 L323 R324 K325 T326 D327 P328 R329 Y330 T331 C332 Q333 R334 E335 F336 A337 L338 K339 H340 L341 P342 G343 D344 P345 M346 F347 K348 L349 V350 A351 Q352 L353 Y354 K355 I356 V357 P358 N359 V360 L361 L362 E363 Q364 A367 A368 N369 P370 W371 P372 N373 V374 D375 A376 H377 S378
G379 V380 L381 L382 Q383 Y384 Y385 G386 M387 T388 E389 H390 N391 Y392 Y393 T394 V395 L396 F397 S400 R401 A402 L403 G404 V405 L406 A407 Q408 L409 T410 W411 S412 R413 A414 L415 G416 F417 E420 R421 P422 K423 S424 M425 S426 T427 D428 G429 L430 I431 A432 L433

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	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^2)	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(^{o})	Ideal(^{o})
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 (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	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%)	2 4
2	B	423/429 (99%)	325 (77%)	72 (17%)	26 (6%)	2 5
All	All	846/862 (98%)	644 (76%)	149 (18%)	53 (6%)	2 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 (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)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.