



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:05 pm BST

PDB ID : 1A59
Title : COLD-ACTIVE CITRATE SYNTHASE
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Deposited on : 1998-02-20
Resolution : 2.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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
buster-report	:	1.1.7 (2018)
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)	:	2.11

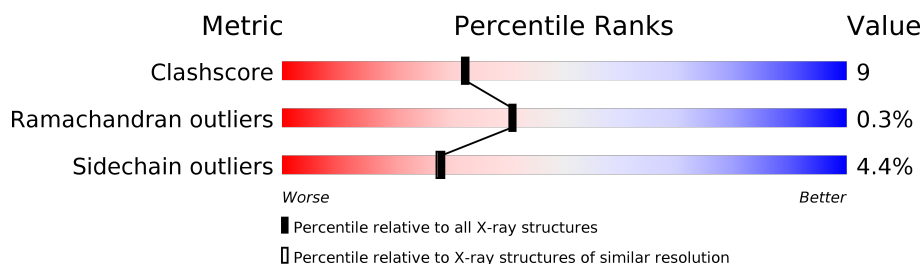
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	378	

2 Entry composition [i](#)

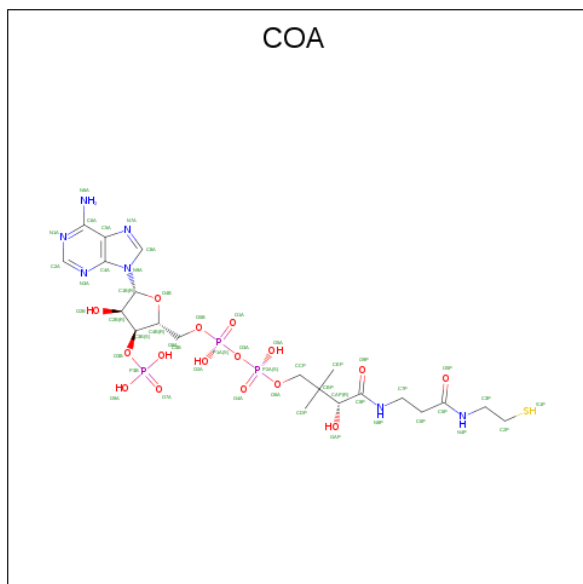
There are 3 unique types of molecules in this entry. The entry contains 2951 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	377	2892	1821	505	550	16	0	0	0

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	46	20	7	16	3	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



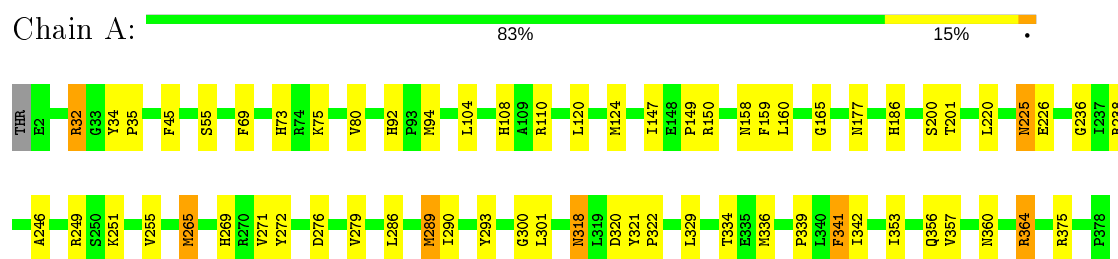
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

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 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: CITRATE SYNTHASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	70.80 Å 70.80 Å 307.80 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.09	Depositor
% Data completeness (in resolution range)	96.2 (100.00-2.09)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.184 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2951	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, CIT

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	0.34	0/2954	0.60	0/4006

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2892	0	2815	51	0
2	A	46	0	27	1	0
3	A	13	0	5	2	0
All	All	2951	0	2847	51	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 9.

All (51) 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:200:SER:HA	1:A:360:ASN:HD21	1.21	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:PHE:H	1:A:177:ASN:HD21	1.18	0.88
1:A:32:ARG:HD3	1:A:55:SER:HA	1.57	0.86
1:A:110:ARG:HH11	1:A:110:ARG:HG2	1.53	0.73
1:A:225:ASN:HD22	1:A:226:GLU:N	1.89	0.71
1:A:269:HIS:HD2	1:A:271:VAL:H	1.37	0.70
1:A:108:HIS:CD2	1:A:110:ARG:H	2.10	0.69
1:A:200:SER:HA	1:A:360:ASN:ND2	2.04	0.69
1:A:276:ASP:HB3	1:A:279:VAL:HG23	1.74	0.68
1:A:225:ASN:HD22	1:A:226:GLU:H	1.42	0.67
1:A:356:GLN:HE21	1:A:360:ASN:ND2	1.94	0.66
1:A:92:HIS:HD2	1:A:94:MET:H	1.41	0.66
1:A:45:PHE:N	1:A:177:ASN:HD21	1.91	0.65
1:A:150:ARG:H	1:A:158:ASN:ND2	1.94	0.64
1:A:356:GLN:HE21	1:A:360:ASN:HD22	1.44	0.62
1:A:186:HIS:HD2	3:A:379:CIT:O1	1.83	0.61
1:A:108:HIS:HD2	1:A:110:ARG:H	1.47	0.60
1:A:269:HIS:CD2	1:A:271:VAL:H	2.20	0.59
1:A:45:PHE:H	1:A:177:ASN:ND2	1.96	0.57
1:A:147:ILE:HD13	1:A:165:GLY:HA2	1.87	0.56
1:A:92:HIS:CD2	1:A:94:MET:H	2.23	0.54
1:A:186:HIS:HE1	1:A:272:TYR:OH	1.90	0.54
1:A:110:ARG:NH1	1:A:110:ARG:HG2	2.18	0.53
1:A:246:ALA:HB1	1:A:300:GLY:C	2.30	0.52
1:A:69:PHE:O	1:A:73:HIS:HD2	1.95	0.50
1:A:318:ASN:HD22	1:A:320:ASP:H	1.60	0.49
1:A:290:ILE:HD13	1:A:329:LEU:HD11	1.95	0.48
1:A:265:MET:CE	2:A:380:COA:H72	2.45	0.47
1:A:289:MET:HA	1:A:289:MET:CE	2.44	0.47
1:A:286:LEU:O	1:A:290:ILE:HG12	2.15	0.47
1:A:251:LYS:O	1:A:255:VAL:HG23	2.15	0.47
1:A:120:LEU:O	1:A:124:MET:HG3	2.15	0.47
1:A:149:PRO:HA	1:A:158:ASN:HD21	1.80	0.46
1:A:236:GLY:H	1:A:249:ARG:HH12	1.64	0.46
1:A:276:ASP:HB3	1:A:279:VAL:CG2	2.43	0.46
1:A:150:ARG:H	1:A:158:ASN:HD21	1.64	0.46
1:A:108:HIS:HD2	1:A:110:ARG:N	2.14	0.45
1:A:269:HIS:HE1	3:A:379:CIT:O7	2.00	0.44
1:A:236:GLY:N	1:A:249:ARG:HH12	2.14	0.44
1:A:289:MET:HG3	1:A:293:TYR:CE2	2.53	0.44
1:A:226:GLU:HG3	1:A:334:THR:HG22	1.99	0.43
1:A:147:ILE:HD13	1:A:165:GLY:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:O	1:A:357:VAL:HG23	2.18	0.43
1:A:336:MET:C	1:A:339:PRO:HD2	2.38	0.43
1:A:80:VAL:HG21	1:A:104:LEU:HG	2.01	0.42
1:A:341:PHE:HD1	1:A:341:PHE:O	2.02	0.42
1:A:364:ARG:O	1:A:364:ARG:HG3	2.18	0.42
1:A:321:TYR:HB3	1:A:322:PRO:CD	2.49	0.41
1:A:34:TYR:HA	1:A:35:PRO:HD3	1.91	0.41
1:A:75:LYS:HE2	1:A:75:LYS:HB3	1.79	0.41
1:A:94:MET:SD	1:A:342:ILE:HD11	2.62	0.40

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	375/378 (99%)	365 (97%)	9 (2%)	1 (0%)	41	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	ARG

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	298/309 (96%)	285 (96%)	13 (4%)	28	28

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	159	PHE
1	A	160	LEU
1	A	201	THR
1	A	220	LEU
1	A	225	ASN
1	A	265	MET
1	A	289	MET
1	A	301	LEU
1	A	318	ASN
1	A	341	PHE
1	A	364	ARG
1	A	375	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	73	HIS
1	A	92	HIS
1	A	108	HIS
1	A	158	ASN
1	A	177	ASN
1	A	186	HIS
1	A	189	ASN
1	A	225	ASN
1	A	269	HIS
1	A	318	ASN
1	A	360	ASN

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 ⓘ

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$
2	COA	A	380	-	40,48,50	1.93	9 (22%)	51,73,75	1.34	4 (7%)
3	CIT	A	379	-	3,12,12	3.38	2 (66%)	3,17,17	3.09	2 (66%)

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
2	COA	A	380	-	-	10/42/62/64	0/3/3/3
3	CIT	A	379	-	-	4/6/16/16	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	380	COA	P3B-O3B	6.84	1.72	1.59
3	A	379	CIT	C4-C3	-4.93	1.47	1.54
2	A	380	COA	C8A-N7A	4.06	1.41	1.34
2	A	380	COA	C3P-N4P	3.62	1.52	1.45
2	A	380	COA	C5A-N7A	-3.57	1.26	1.39
2	A	380	COA	P3B-O7A	3.46	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	379	CIT	C2-C3	3.08	1.59	1.54
2	A	380	COA	O4B-C1B	2.59	1.44	1.41
2	A	380	COA	C2A-N3A	2.49	1.36	1.32
2	A	380	COA	O9P-C9P	2.13	1.27	1.23
2	A	380	COA	P1A-O5B	2.07	1.67	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	380	COA	C4A-C5A-N7A	4.63	114.23	109.40
3	A	379	CIT	C3-C4-C5	-4.37	107.99	114.98
2	A	380	COA	C1B-N9A-C4A	-4.02	119.57	126.64
2	A	380	COA	N6A-C6A-N1A	3.17	125.15	118.57
3	A	379	CIT	C4-C3-C2	3.01	117.37	109.33
2	A	380	COA	P2A-O3A-P1A	-2.17	125.38	132.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

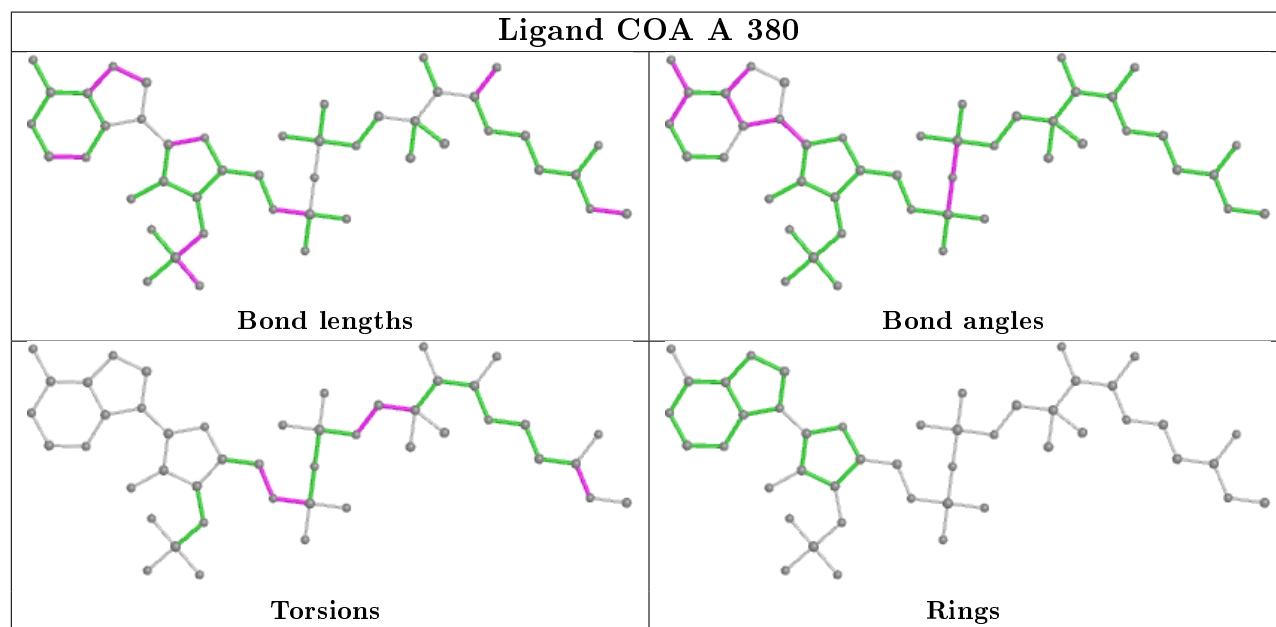
Mol	Chain	Res	Type	Atoms
2	A	380	COA	C5B-O5B-P1A-O1A
2	A	380	COA	C5B-O5B-P1A-O2A
2	A	380	COA	CDP-CBP-CCP-O6A
2	A	380	COA	CEP-CBP-CCP-O6A
2	A	380	COA	CAP-CBP-CCP-O6A
2	A	380	COA	C6P-C5P-N4P-C3P
2	A	380	COA	O5P-C5P-N4P-C3P
3	A	379	CIT	C1-C2-C3-O7
3	A	379	CIT	O7-C3-C4-C5
3	A	379	CIT	C2-C3-C4-C5
3	A	379	CIT	C1-C2-C3-C6
2	A	380	COA	C5B-O5B-P1A-O3A
2	A	380	COA	CBP-CCP-O6A-P2A
2	A	380	COA	C4B-C5B-O5B-P1A

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	380	COA	1	0
3	A	379	CIT	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.