W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:37 PM GMT

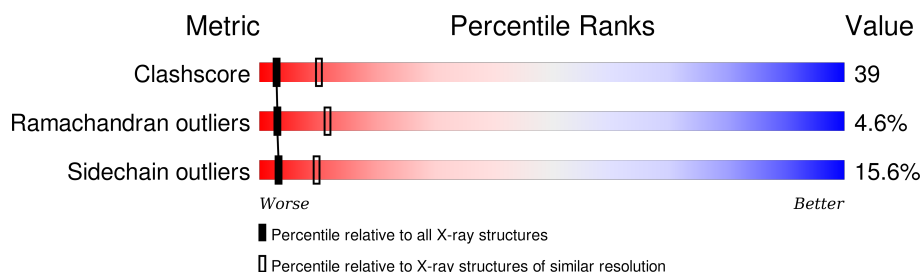|		
PDB ID	:	4CTS
Title	:	CRYSTAL STRUCTURE ANALYSIS AND MOLECULAR MODEL OF A COMPLEX OF CITRATE SYNTHASE WITH OXALOACETATE AND S-ACETONYL-COENZYME A
Authors	:	Remington, S.; Wiegand, G.; Huber, R.
Deposited on	:	1984-01-27
Resolution	:	2.90 Å(reported)

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 2.90 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	Percentile Ranks	Value
Clashscore		39
Ramachandran outliers		4.6%
Sidechain outliers		15.6%

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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	437	30% 41% 23% 6%
1	B	437	32% 40% 22% 7%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7002 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	437	Total 3444	C 2200	N 591	O 634	S 19	227	0	0
1	B	437	Total 3444	C 2200	N 591	O 634	S 19	230	0	0

- Molecule 2 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).
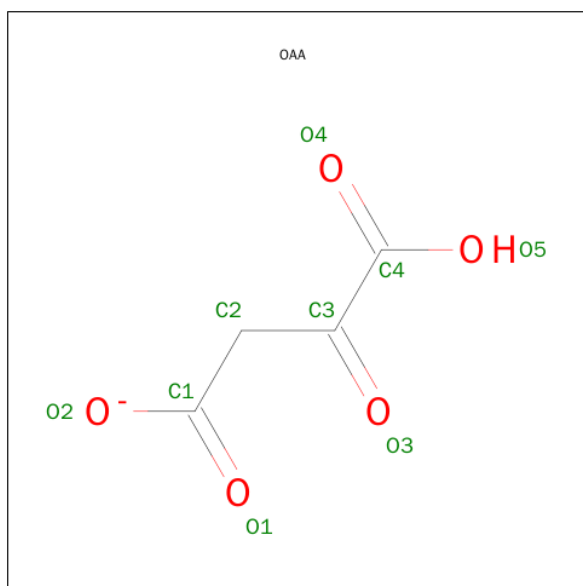
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 9	C 4	O 5	0	0
2	B	1	Total 9	C 4	O 5	0	0

- Molecule 3 is water.

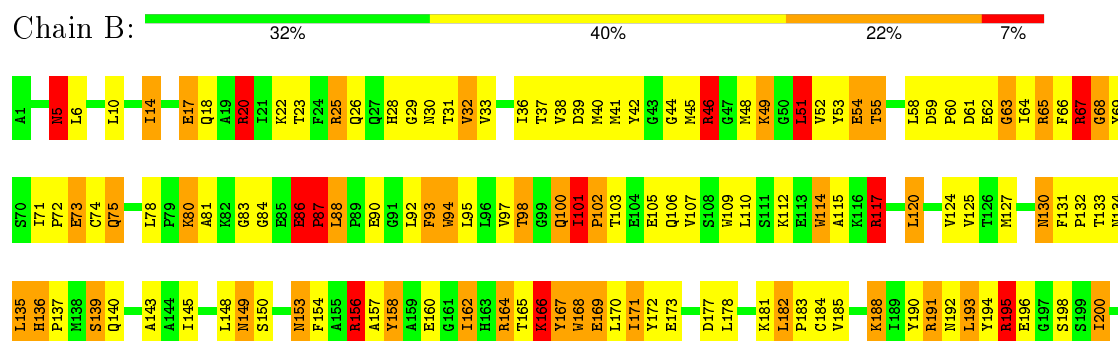| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total 49	O 49	0	0
3	B	47	Total 47	O 47	0	0

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 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 1: CITRATE SYNTHASE

Chain B:

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 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.54Å 101.54Å 224.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7002	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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

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	1.22	11/3528 (0.3%)	1.77	41/4786 (0.9%)
1	B	1.22	11/3528 (0.3%)	1.77	54/4786 (1.1%)
All	All	1.22	22/7056 (0.3%)	1.77	95/9572 (1.0%)

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	1	105
1	B	2	104
All	All	3	209

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	TRP	NE1-CE2	-8.77	1.26	1.37
1	B	109	TRP	NE1-CE2	-8.18	1.26	1.37
1	A	114	TRP	NE1-CE2	-7.93	1.27	1.37
1	A	168	TRP	NE1-CE2	-7.85	1.27	1.37
1	A	371	TRP	NE1-CE2	-7.65	1.27	1.37

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ARG	NE-CZ-NH2	-17.05	111.78	120.30
1	B	65	ARG	NE-CZ-NH1	14.64	127.62	120.30
1	A	191	ARG	NE-CZ-NH2	-11.17	114.72	120.30
1	A	67	ARG	NE-CZ-NH1	-10.86	114.87	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	20	ARG	NE-CZ-NH2	-9.80	115.40	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	37	THR	CB
1	B	37	THR	CB
1	B	307	ASN	CA

5 of 209 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ALA	Mainchain
1	A	18	GLN	Sidechain
1	A	25	ARG	Sidechain
1	A	26	GLN	Sidechain
1	A	32	VAL	Mainchain

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	3444	0	3436	291	17
1	B	3444	0	3436	283	27
2	A	9	0	2	0	0
2	B	9	0	2	0	0
3	A	49	0	0	4	0
3	B	47	0	0	0	2
All	All	7002	0	6876	502	38

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 39.

The worst 5 of 502 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:268:GLY:HA2	1:B:251:VAL:HG13	1.47	0.96
1:A:419:LEU:HD11	1:B:243:VAL:HG22	1.51	0.92
1:B:58:LEU:HD12	1:B:63:GLY:HA2	1.53	0.90
1:A:280:GLU:HA	1:A:283:VAL:HB	1.54	0.90
1:A:75:GLN:HA	1:A:87:PRO:HG3	1.56	0.88

The worst 5 of 38 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:203:ILE:O	3:B:476:HOH:O[6_455]	0.90	1.30
1:B:153:ASN:OD1	1:B:306:TRP:CH2[3_544]	0.98	1.22
1:A:206:LYS:CD	1:B:191:ARG:NH2[6_455]	1.22	0.98
1:B:156:ARG:CZ	1:B:303:ASP:CB[3_544]	1.41	0.79
1:B:153:ASN:CG	1:B:306:TRP:CH2[3_544]	1.42	0.78

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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	435/437 (100%)	359 (82%)	55 (13%)	21 (5%)	3	10
1	B	435/437 (100%)	357 (82%)	59 (14%)	19 (4%)	3	12
All	All	870/874 (100%)	716 (82%)	114 (13%)	40 (5%)	3	11

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	LYS
1	A	205	SER
1	A	239	GLU
1	B	166	LYS
1	B	239	GLU

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	371/371 (100%)	311 (84%)	60 (16%)	3	9
1	B	371/371 (100%)	315 (85%)	56 (15%)	3	11
All	All	742/742 (100%)	626 (84%)	116 (16%)	3	10

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	359	ASN
1	B	49	LYS
1	B	394	THR
1	A	373	ASN
1	A	421	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	383	GLN
1	B	30	ASN
1	B	359	ASN
1	A	391	ASN
1	B	5	ASN

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.

wwPDB X-ray Structure Validation Summary Report

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	#$|Z| > 2$
2	OAA	A	438	-	2,8,8	1.28	0	2,10,10	1.97	1 (50%)
2	OAA	B	438	-	2,8,8	2.02	1 (50%)	2,10,10	1.07	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
2	OAA	A	438	-	-	0/2/8/8	0/0/0/0
2	OAA	B	438	-	-	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)
2	B	438	OAA	O3-C3	2.65	1.26	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	438	OAA	C1-C2-C3	-2.78	110.46	115.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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