



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:01 AM UTC

PDB ID : 4CTS / pdb_00004cts
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)

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

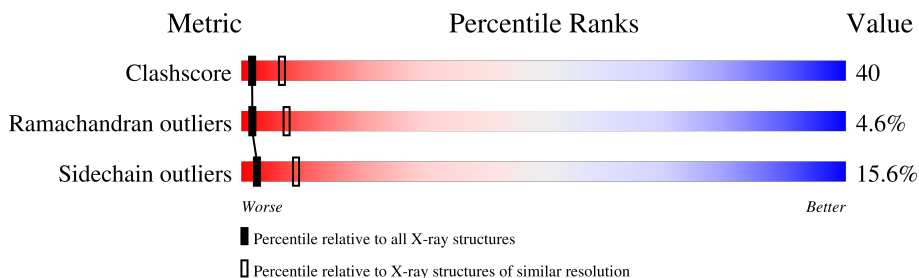
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 of 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	437	 22% 38% 29% 11%
1	B	437	 23% 38% 28% 11%

2 Entry composition [i](#)

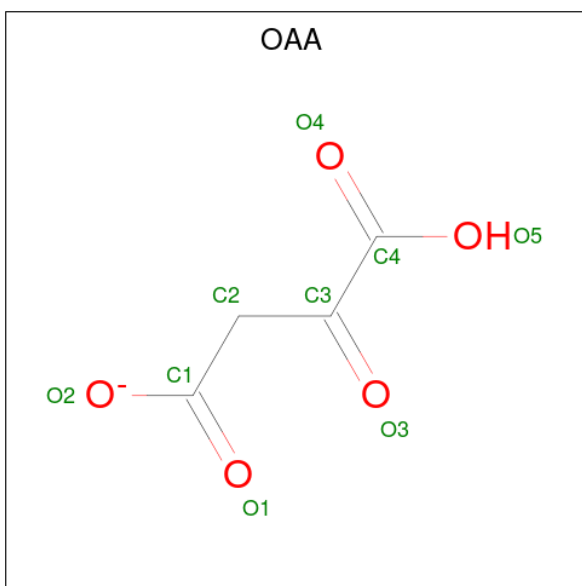
There are 3 unique types of molecules in this entry. The entry contains 7002 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
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 (CCD ID: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
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.

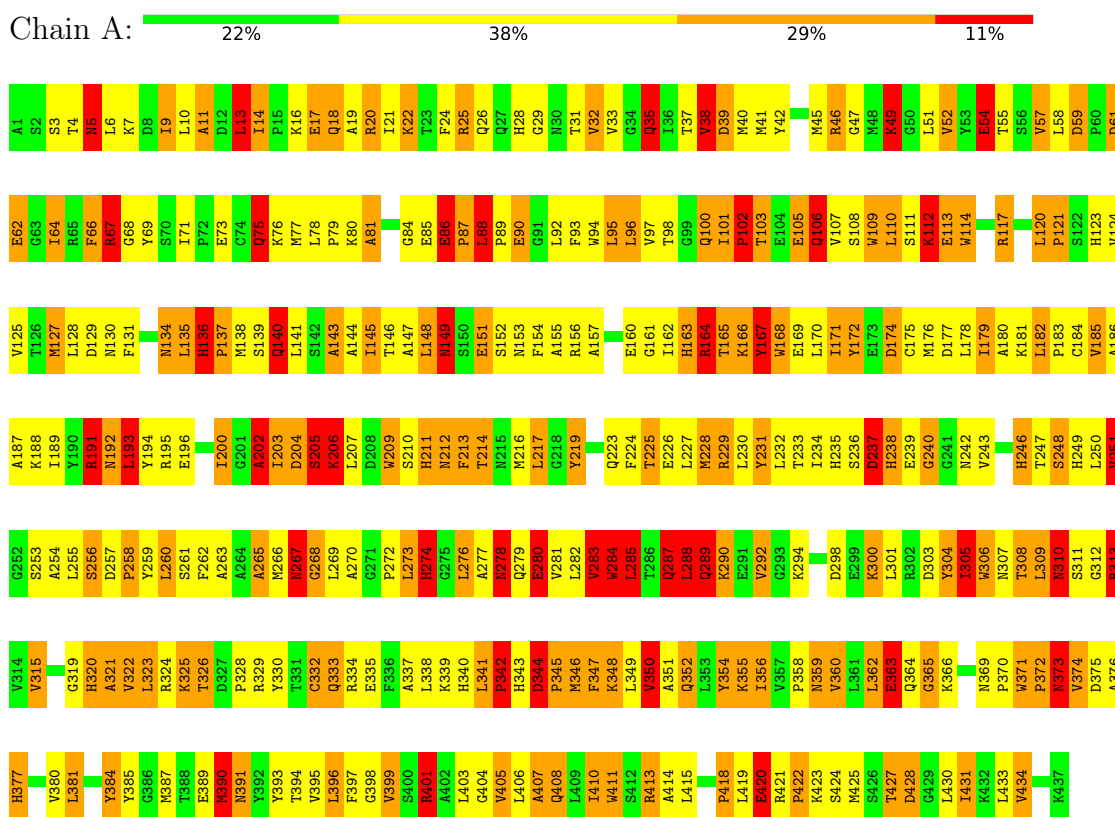
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total 49	O 49	0	0
3	B	47	Total 47	O 47	0	0

3 Residue-property plots

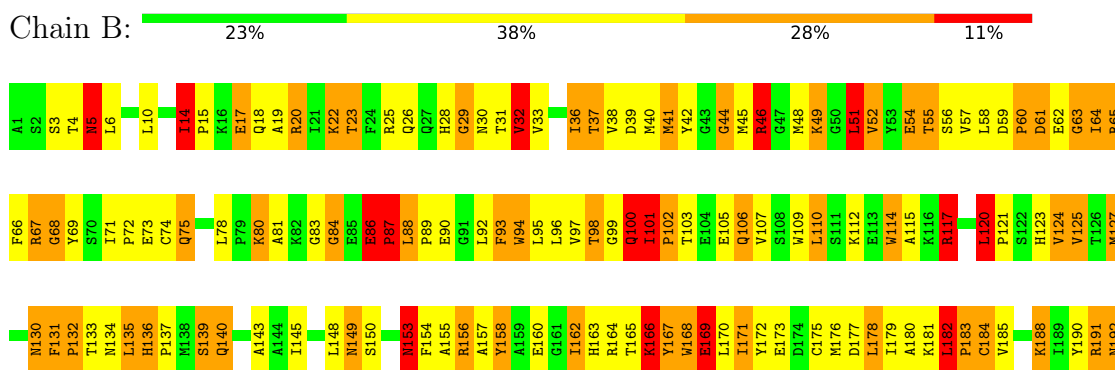
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: CITRATE SYNTHASE



L183	L194	R195	E196	G197	S198	S199	I200	I203	D204	S205	K206	L207	D208	W209	S210	H211	N212	F213	T214	M215	M216	L217	G218	Y219	T220	D221	A222	Q223	F224	T225	E226	L227	M228	R229	L230	Y231	L232	H235	S236	D237	H238	E239	N242	V243	S244	A245	H246	T247	S248	H249	L250	V251	G252	S253	A254	L255	
S256	D257	P258	Y259	L260	S261	F262	A263	A264	A265	M266	V267	A270	G271	P272	L273	H274	G275	L276	A277	N278	Q279	E280	V281	L282	V283	W284	L285	T286	Q287	L288	Q289	K290	E291	V292	G293	K294	D295	V296	S297	D298	E299	K300	L301	R302	D303	Y304	I305	W306	M307	T308	L309	N310	S311	G312	R313	V314	P316
G317	Y318	G319	R320	A321	W322	L323	R324	R325	T326	D327	P328	R329	Y330	T331	C332	Q333	R334	E335	F336	A337	L338	K339	H340	I341	P342	H343	D344	P345	M346	F347	K348	L349	V350	Y354	K355	I356	V357	P358	N359	L362	E363	Q364	G365	K366	A367	K368	N369	P370	W371	P372	N373	V374	D375	A376	H377	S378	G379
V380	L381	L382	Q383	Y384	Y385	G386	M387	T388	E389	M390	N391	Y392	Y393	T394	V395	L396	F397	G398	V399	S400	R401	G404	V405	Q408	L409	W410	W411	S412	R413	A414	F417	P418	L419	E420	R421	P422	K423	S424	M425	S426	T427	D428	G429	L430	I431	K432	L433	V434	K437								

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore 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.	Xtrriage
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	1.67	42/3528 (1.2%)	2.37	213/4786 (4.5%)
1	B	1.67	50/3528 (1.4%)	2.39	241/4786 (5.0%)
All	All	1.67	92/7056 (1.3%)	2.38	454/9572 (4.7%)

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 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	340	HIS	CE1-NE2	10.89	1.43	1.32
1	B	211	HIS	ND1-CE1	10.52	1.43	1.32
1	B	274	HIS	ND1-CE1	10.47	1.43	1.32
1	A	340	HIS	CE1-NE2	10.44	1.43	1.32
1	A	377	HIS	CE1-NE2	10.31	1.42	1.32

The worst 5 of 454 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	GLY	CA-C-N	13.22	133.94	122.17
1	B	83	GLY	C-N-CA	13.22	133.94	122.17
1	A	28	HIS	CA-CB-CG	-11.28	102.52	113.80
1	B	28	HIS	CA-CB-CG	-10.74	103.06	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	ILE	N-CA-C	10.29	120.23	111.90

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	297	17
1	B	3444	0	3436	297	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	518	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 40.

The worst 5 of 518 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:127:MET:HE3	1:B:127:MET:HE3	1.41	0.99
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

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 [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	435/437 (100%)	359 (82%)	55 (13%)	21 (5%)	2 7
1	B	435/437 (100%)	357 (82%)	59 (14%)	19 (4%)	2 8
All	All	870/874 (100%)	716 (82%)	114 (13%)	40 (5%)	2 7

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%)	2 8
1	B	371/371 (100%)	315 (85%)	56 (15%)	3 10
All	All	742/742 (100%)	626 (84%)	116 (16%)	2 9

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

Mol	Chain	Res	Type
1	A	405	VAL
1	B	405	VAL
1	B	110	LEU
1	B	399	VAL
1	B	315	VAL

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

Mol	Chain	Res	Type
1	B	267	ASN
1	B	279	GLN
1	B	391	ASN
1	A	274	HIS
1	A	267	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.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	B	438	-	8,8,8	3.81	2 (25%)	8,10,10	1.62	2 (25%)
2	OAA	A	438	-	8,8,8	4.12	1 (12%)	8,10,10	1.37	1 (12%)

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	B	438	-	-	1/8/8/8	-
2	OAA	A	438	-	-	2/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	438	OAA	C3-C4	-11.21	1.36	1.53
2	B	438	OAA	C3-C4	-10.08	1.38	1.53
2	B	438	OAA	O5-C4	-2.03	1.25	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	438	OAA	O5-C4-C3	2.60	120.80	113.59
2	A	438	OAA	O2-C1-O1	-2.35	117.28	123.33
2	B	438	OAA	O5-C4-O4	-2.25	118.53	123.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	438	OAA	C1-C2-C3-O3
2	A	438	OAA	C1-C2-C3-O3
2	A	438	OAA	C1-C2-C3-C4

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

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.