



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 04:02 pm BST

PDB ID : 1S5O
Title : Structural and Mutational Characterization of L-carnitine Binding to Human carnitine Acetyltransferase
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Deposited on : 2004-01-21
Resolution : 1.80 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

<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**
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

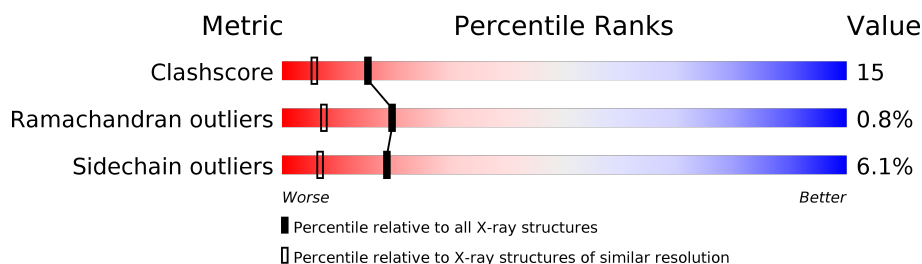
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 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	616	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5190 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.

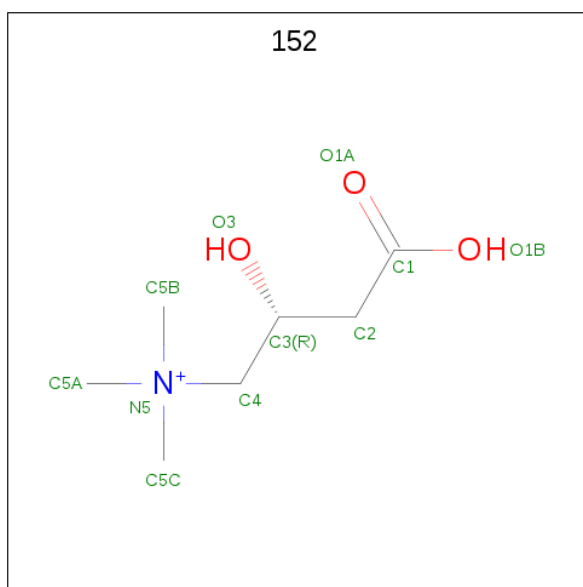
- Molecule 1 is a protein called carnitine acetyltransferase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	0	0
			4714	3006	810	872	26			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP P43155
A	2	ARG	-	CLONING ARTIFACT	UNP P43155
A	3	GLY	-	CLONING ARTIFACT	UNP P43155
A	4	SER	-	CLONING ARTIFACT	UNP P43155
A	5	HIS	-	CLONING ARTIFACT	UNP P43155
A	6	HIS	-	CLONING ARTIFACT	UNP P43155
A	7	HIS	-	CLONING ARTIFACT	UNP P43155
A	8	HIS	-	CLONING ARTIFACT	UNP P43155
A	9	HIS	-	CLONING ARTIFACT	UNP P43155
A	10	HIS	-	CLONING ARTIFACT	UNP P43155
A	11	THR	-	CLONING ARTIFACT	UNP P43155
A	12	ASP	-	CLONING ARTIFACT	UNP P43155
A	13	PRO	-	CLONING ARTIFACT	UNP P43155
A	513	THR	MET	SEE REMARK 999	UNP P43155
A	606	ILE	-	CLONING ARTIFACT	UNP P43155
A	607	SER	-	CLONING ARTIFACT	UNP P43155
A	608	GLU	-	CLONING ARTIFACT	UNP P43155
A	609	GLU	-	CLONING ARTIFACT	UNP P43155
A	610	ASP	-	CLONING ARTIFACT	UNP P43155
A	611	LEU	-	CLONING ARTIFACT	UNP P43155
A	612	SER	-	CLONING ARTIFACT	UNP P43155
A	613	LEU	-	CLONING ARTIFACT	UNP P43155
A	614	ILE	-	CLONING ARTIFACT	UNP P43155
A	615	SER	-	CLONING ARTIFACT	UNP P43155
A	616	GLY	-	CLONING ARTIFACT	UNP P43155

- Molecule 2 is CARNITINE (three-letter code: 152) (formula: C₇H₁₆NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 3 is water.

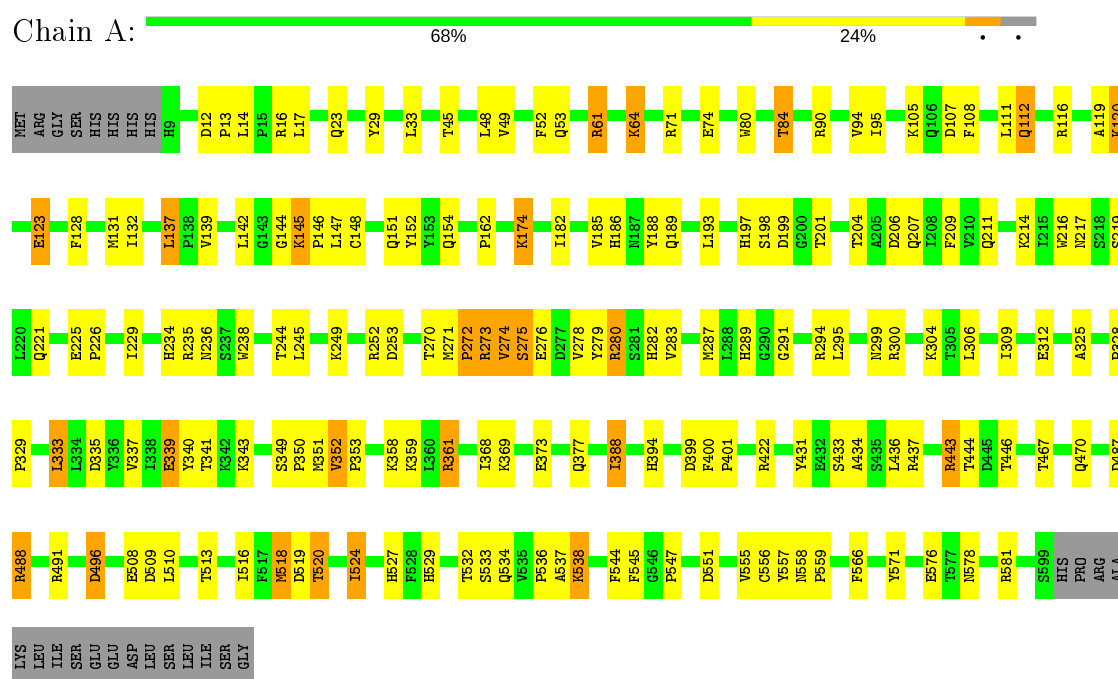
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	465	Total	O	0	0
			465	465		

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: carnitine acetyltransferase isoform 2



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.56Å 84.65Å 57.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS, SHELXL-97	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5190	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: 152

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	0.36	0/4829	1.04	15/6550 (0.2%)

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	1	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	61	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	A	90	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	361	ARG	CD-NE-CZ	7.59	134.22	123.60
1	A	61	ARG	CD-NE-CZ	7.39	133.94	123.60
1	A	443	ARG	NE-CZ-NH1	6.45	123.52	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	520	THR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	519	ASP	Peptide

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	4714	0	4689	140	11
2	A	11	0	15	1	0
3	A	465	0	0	23	11
All	All	5190	0	4704	141	16

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 15.

The worst 5 of 141 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:275:SER:O	1:A:276:GLU:CG	1.79	1.30
1:A:275:SER:O	1:A:276:GLU:HG2	1.10	1.28
1:A:467:THR:HG23	1:A:470:GLN:HE21	1.43	0.84
1:A:278:VAL:HG12	1:A:282:HIS:CD2	2.12	0.83
1:A:274:VAL:HG11	1:A:279:TYR:HA	1.63	0.81

The worst 5 of 16 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:294:ARG:CZ	3:A:744:HOH:O[2_565]	0.24	1.96
1:A:273:ARG:NE	1:A:520:THR:CG2[2_565]	0.94	1.26
1:A:294:ARG:NH1	3:A:744:HOH:O[2_565]	1.23	0.97
1:A:294:ARG:NE	3:A:744:HOH:O[2_565]	1.34	0.86
1:A:294:ARG:NH2	3:A:744:HOH:O[2_565]	1.47	0.73

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	589/616 (96%)	569 (97%)	15 (2%)	5 (1%)	19 7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	SER
1	A	520	THR
1	A	273	ARG
1	A	272	PRO
1	A	274	VAL

5.3.2 Protein sidechains ⓘ

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	521/543 (96%)	489 (94%)	32 (6%)	18 7

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	LYS
1	A	339	GLU
1	A	538	LYS
1	A	333	LEU
1	A	351	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	HIS
1	A	299	ASN
1	A	529	HIS
1	A	236	ASN

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Mol	Chain	Res	Type
1	A	527	HIS

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 ⓘ

1 ligand is 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	152	A	617	-	7,10,10	1.01	0	10,14,14	1.54	2 (20%)

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	152	A	617	-	-	0/7/9/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	617	152	C3-C4-N5	-4.22	109.61	116.83
2	A	617	152	O3-C3-C2	-2.20	104.91	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	617	152	1	0

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.