



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 12:03 PM EDT

PDB ID : 5O1P / pdb_00005o1p
Title : Crystal structure of human aminoadipate semialdehyde synthase, saccharopine dehydrogenase.
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Deposited on : 2017-05-18
Resolution : 1.90 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 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)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

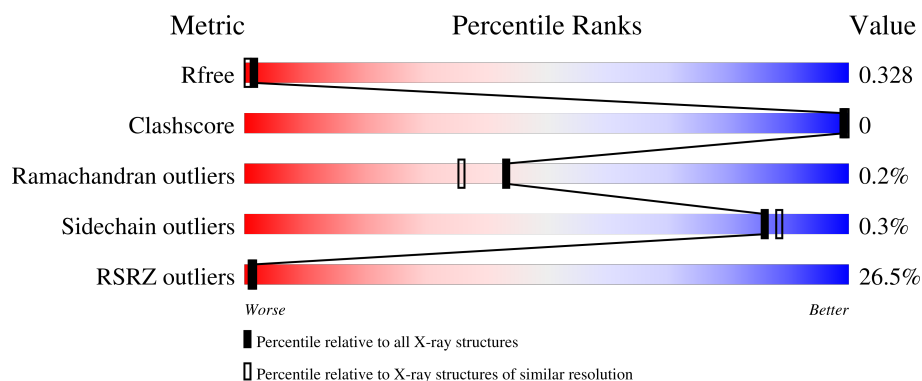
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	497	24% 88% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3371 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 Alpha-aminoadipic semialdehyde synthase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3325	2124	543	638	20	0	1	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	430	MET	-	initiating methionine	UNP Q9UDR5
A	431	GLY	-	expression tag	UNP Q9UDR5
A	432	HIS	-	expression tag	UNP Q9UDR5
A	433	HIS	-	expression tag	UNP Q9UDR5
A	434	HIS	-	expression tag	UNP Q9UDR5
A	435	HIS	-	expression tag	UNP Q9UDR5
A	436	HIS	-	expression tag	UNP Q9UDR5
A	437	HIS	-	expression tag	UNP Q9UDR5
A	438	SER	-	expression tag	UNP Q9UDR5
A	439	SER	-	expression tag	UNP Q9UDR5
A	440	GLY	-	expression tag	UNP Q9UDR5
A	441	VAL	-	expression tag	UNP Q9UDR5
A	442	ASP	-	expression tag	UNP Q9UDR5
A	443	LEU	-	expression tag	UNP Q9UDR5
A	444	GLY	-	expression tag	UNP Q9UDR5
A	445	THR	-	expression tag	UNP Q9UDR5
A	446	GLU	-	expression tag	UNP Q9UDR5
A	447	ASN	-	expression tag	UNP Q9UDR5
A	448	LEU	-	expression tag	UNP Q9UDR5
A	449	TYR	-	expression tag	UNP Q9UDR5
A	450	PHE	-	expression tag	UNP Q9UDR5
A	451	GLN	-	expression tag	UNP Q9UDR5
A	452	SER	-	expression tag	UNP Q9UDR5
A	453	MET	-	expression tag	UNP Q9UDR5
A	454	ALA	-	expression tag	UNP Q9UDR5
A	615	SER	THR	conflict	UNP Q9UDR5

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.46Å 91.46Å 150.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 1.90 49.03 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.03-1.90) 100.0 (49.03-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.311 , 0.323 0.318 , 0.328	Depositor DCC
R_{free} test set	2554 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3371	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.56	0/3387	0.77	0/4598

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	3325	0	3315	2	0
2	A	8	0	12	0	0
3	A	12	0	18	0	0
4	A	26	0	0	0	0
All	All	3371	0	3345	2	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 0.

All (2) 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:633:CYS:SG	1:A:634:GLY:N	2.70	0.63
1:A:608:ASP:HA	1:A:838:MET:HE1	1.97	0.45

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	439/497 (88%)	419 (95%)	19 (4%)	1 (0%)	43 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	898	PRO

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	355/418 (85%)	354 (100%)	1 (0%)	86 88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	636	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	516	GLN
1	A	547	GLN
1	A	793	GLN
1	A	853	HIS

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](#)

5 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	EDO	A	1001	-	3,3,3	0.42	0	2,2,2	0.37	0
3	DMS	A	1005	-	3,3,3	0.57	0	3,3,3	0.51	0
3	DMS	A	1004	-	3,3,3	0.57	0	3,3,3	0.53	0
3	DMS	A	1003	-	3,3,3	0.57	0	3,3,3	0.53	0
2	EDO	A	1002	-	3,3,3	0.43	0	2,2,2	0.33	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	EDO	A	1001	-	-	1/1/1/1	-
2	EDO	A	1002	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	EDO	O1-C1-C2-O2
2	A	1002	EDO	O1-C1-C2-O2

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/497 (88%)	1.55	117 (26%) 1 1	13, 81, 113, 135	1 (0%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	787	LEU	8.9
1	A	533	ILE	5.7
1	A	926	PRO	5.4
1	A	490	TYR	4.9
1	A	633	CYS	4.5
1	A	782	ALA	4.4
1	A	755	ALA	4.3
1	A	778	VAL	4.2
1	A	772	PRO	4.2
1	A	544	VAL	4.2
1	A	634	GLY	3.9
1	A	576	ALA	3.7
1	A	517	ILE	3.7
1	A	575	THR	3.7
1	A	582	ALA	3.6
1	A	924	ILE	3.6
1	A	529	VAL	3.6
1	A	542	PHE	3.6
1	A	788	GLY	3.5
1	A	567	ILE	3.5
1	A	750	ALA	3.5
1	A	597	ILE	3.4
1	A	786	LYS	3.4
1	A	659	MET	3.4
1	A	487	GLY	3.3
1	A	779	LEU	3.3
1	A	520	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	657	VAL	3.2
1	A	768	VAL	3.2
1	A	543	LEU	3.2
1	A	491	ILE	3.2
1	A	488	SER	3.1
1	A	541	GLY	3.1
1	A	586	LEU	3.1
1	A	658	LEU	3.1
1	A	568	THR	3.1
1	A	535	LYS	3.1
1	A	531	MET	3.1
1	A	783	VAL	3.0
1	A	595	ILE	3.0
1	A	789	GLY	3.0
1	A	673	VAL	3.0
1	A	540	LEU	2.9
1	A	891	GLY	2.9
1	A	545	ALA	2.9
1	A	509	VAL	2.8
1	A	925	LYS	2.8
1	A	534	CYS	2.8
1	A	549	LEU	2.8
1	A	561	LEU	2.8
1	A	524	TYR	2.8
1	A	512	ASP	2.8
1	A	720	LEU	2.7
1	A	578	TYR	2.7
1	A	843	GLY	2.7
1	A	557	VAL	2.7
1	A	706	THR	2.7
1	A	598	ILE	2.7
1	A	864	ILE	2.7
1	A	853	HIS	2.6
1	A	655	VAL	2.6
1	A	652	TRP	2.6
1	A	528	PRO	2.6
1	A	484	LEU	2.6
1	A	777	ASP	2.6
1	A	601	LEU	2.6
1	A	748	LEU	2.5
1	A	758	LEU	2.5
1	A	763	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	903	ILE	2.5
1	A	593	ALA	2.5
1	A	923	THR	2.5
1	A	590	VAL	2.5
1	A	767	LEU	2.4
1	A	584	LYS	2.4
1	A	507	ILE	2.4
1	A	836	ILE	2.4
1	A	917	ILE	2.4
1	A	661	VAL	2.4
1	A	496	LEU	2.4
1	A	602	GLY	2.4
1	A	675	ASN	2.3
1	A	571	VAL	2.3
1	A	574	VAL	2.3
1	A	583	LEU	2.3
1	A	682	PHE	2.3
1	A	539	LYS	2.3
1	A	530	SER	2.3
1	A	564	LYS	2.3
1	A	495	VAL	2.3
1	A	702	ASN	2.3
1	A	811	ALA	2.2
1	A	850	HIS	2.2
1	A	824	MET	2.2
1	A	742	LEU	2.2
1	A	563	ALA	2.2
1	A	485	VAL	2.2
1	A	808	VAL	2.2
1	A	510	GLY	2.2
1	A	565	ALA	2.2
1	A	890	ILE	2.2
1	A	562	VAL	2.2
1	A	822	LEU	2.2
1	A	913	ALA	2.2
1	A	558	LEU	2.1
1	A	898	PRO	2.1
1	A	536	GLN	2.1
1	A	814	ILE	2.1
1	A	757	PRO	2.1
1	A	579	ILE	2.1
1	A	907	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	503	GLY	2.1
1	A	660	ASN	2.1
1	A	784	LEU	2.1
1	A	696	ASN	2.0
1	A	537	GLU	2.0
1	A	526	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DMS	A	1004	4/4	0.75	0.22	119,119,120,120	0
2	EDO	A	1001	4/4	0.76	0.19	86,87,87,88	0
3	DMS	A	1005	4/4	0.80	0.23	115,115,116,116	0
3	DMS	A	1003	4/4	0.81	0.21	136,136,137,137	0
2	EDO	A	1002	4/4	0.88	0.14	92,92,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.