WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:38 PM GMT

PDB ID	:	1PWE
Title	:	Rat Liver L-Serine Dehydratase Apo Enzyme
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Deposited on	:	2003-07-01
Resolution	:	2.80 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

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the ⓘ symbol.

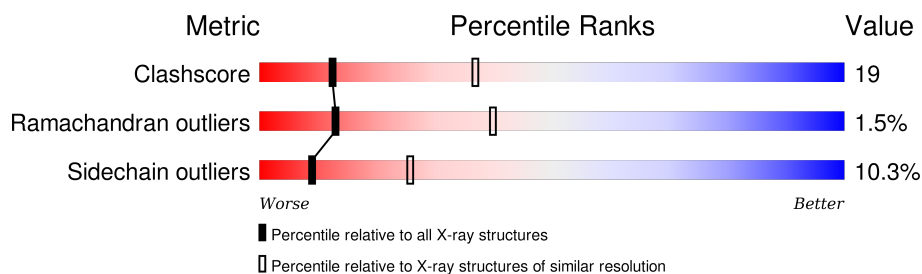The following versions of software and data (see references ⓘ) were used in the production of this report:

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 2.80 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	Percentile Ranks	Value
Clashscore		19
Ramachandran outliers		1.5%
Sidechain outliers		10.3%

Worse   *Better*

■ 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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. 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	327	63% 28% 5% •
1	B	327	61% 31% 5% •
1	C	327	63% 28% 5% •
1	D	327	58% 32% 6% •
1	E	327	61% 30% 6% •
1	F	327	61% 31% 5% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14065 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 L-serine dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total 2326	C 1484	N 395	O 434	S 13	0	0	0
1	B	315	Total 2326	C 1484	N 395	O 434	S 13	0	0	0
1	C	315	Total 2326	C 1484	N 395	O 434	S 13	0	0	0
1	D	315	Total 2326	C 1484	N 395	O 434	S 13	0	0	0
1	E	315	Total 2326	C 1484	N 395	O 434	S 13	0	0	0
1	F	315	Total 2326	C 1484	N 395	O 434	S 13	0	0	0

- Molecule 2 is water.

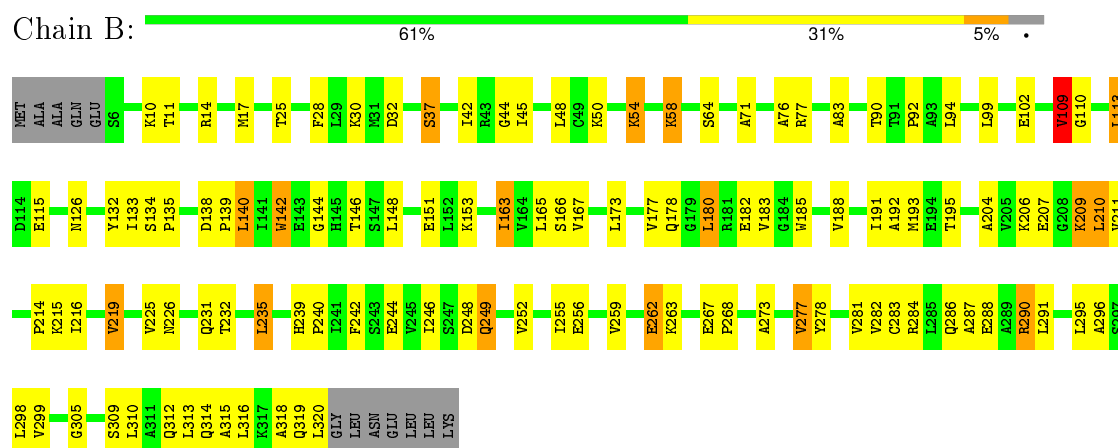| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total 19	O 19	0	0
2	B	22	Total 22	O 22	0	0
2	C	14	Total 14	O 14	0	0
2	D	16	Total 16	O 16	0	0
2	E	16	Total 16	O 16	0	0
2	F	22	Total 22	O 22	0	0

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.
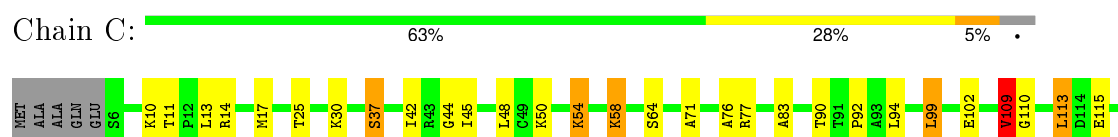
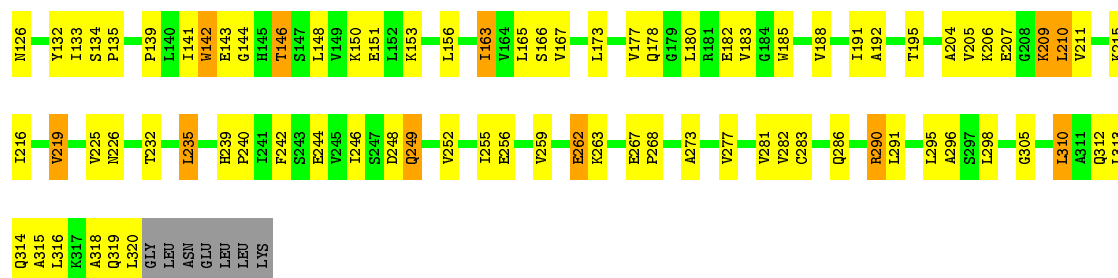Note EDS was not executed.

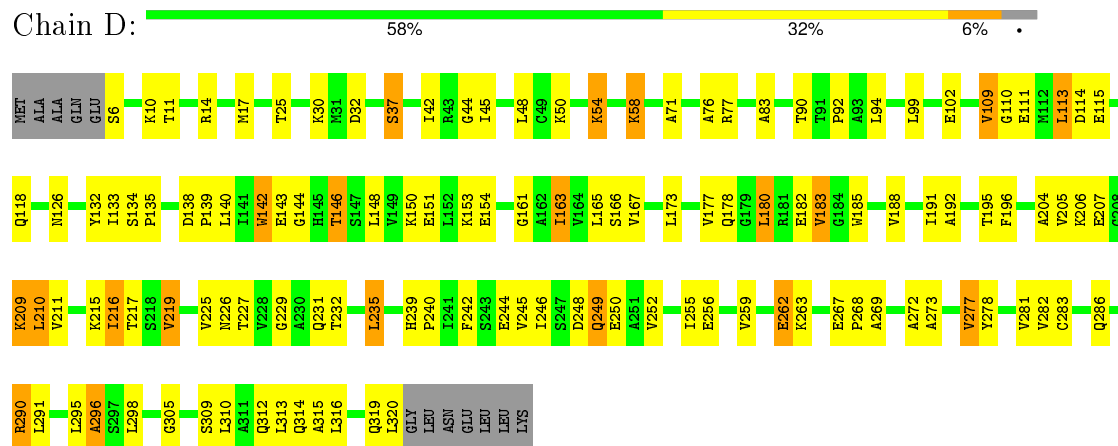- Molecule 1: L-serine dehydratase

- Molecule 1: L-serine dehydratase

- Molecule 1: L-serine dehydratase

• Molecule 1: L-serine dehydratase

Chain D:

• Molecule 1: L-serine dehydratase

Chain E:

• Molecule 1: L-serine dehydratase

Chain F:

I216 V219 V225 N226 T227 T232 L235 E238 H239 P240 I241 F242 S243 E244 V245 I246 S247 D248 Q249 V252 I255 E256 V259 E262 K263 E267 P268 A269 A272 A273 V281 V282 C283 Q286 R290 L291 L295 A296 I301 G305 S309 L310

A311 Q312 L313 Q314 A315 L316 K317 A318 Q319 L320 GLY LEU ASN GLU LEU LEU LYS

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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.63Å 169.84Å 96.00Å 90.00° 92.75° 90.00°	Depositor
Resolution (Å)	23.52 – 2.80	Depositor
% Data completeness (in resolution range)	86.3 (23.52-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14065	wwPDB-VP
Average B, all atoms (Å²)	25.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.45	0/2365	0.64	0/3207
1	B	0.45	0/2365	0.64	0/3207
1	C	0.45	0/2365	0.64	0/3207
1	D	0.46	0/2365	0.65	0/3207
1	E	0.46	0/2365	0.64	0/3207
1	F	0.46	0/2365	0.64	0/3207
All	All	0.45	0/14190	0.64	0/19242

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 (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	2326	0	2415	92	0
1	B	2326	0	2415	95	0
1	C	2326	0	2415	89	0
1	D	2326	0	2415	103	0
1	E	2326	0	2415	97	0
1	F	2326	0	2415	99	0
2	A	19	0	0	0	0
2	B	22	0	0	0	0
2	C	14	0	0	0	0
2	D	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	16	0	0	0	0
2	F	22	0	0	2	0
All	All	14065	0	14490	554	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 19.

The worst 5 of 554 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:C:209:LYS:HG3	1:C:210:LEU:H	1.20	1.07
1:D:209:LYS:HG3	1:D:210:LEU:H	1.25	1.00
1:F:209:LYS:HG3	1:F:210:LEU:H	1.32	0.95
1:C:249:GLN:H	1:C:249:GLN:HE21	1.14	0.94
1:D:249:GLN:HE21	1:D:249:GLN:H	1.15	0.91

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	313/327 (96%)	289 (92%)	19 (6%)	5 (2%)	12	38
1	B	313/327 (96%)	287 (92%)	21 (7%)	5 (2%)	12	38
1	C	313/327 (96%)	288 (92%)	20 (6%)	5 (2%)	12	38
1	D	313/327 (96%)	288 (92%)	21 (7%)	4 (1%)	15	44
1	E	313/327 (96%)	290 (93%)	18 (6%)	5 (2%)	12	38
1	F	313/327 (96%)	289 (92%)	19 (6%)	5 (2%)	12	38
All	All	1878/1962 (96%)	1731 (92%)	118 (6%)	29 (2%)	13	40

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	ARG
1	A	296	ALA
1	B	290	ARG
1	B	296	ALA
1	C	290	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	250/259 (96%)	223 (89%)	27 (11%)	8	23
1	B	250/259 (96%)	223 (89%)	27 (11%)	8	23
1	C	250/259 (96%)	225 (90%)	25 (10%)	9	27
1	D	250/259 (96%)	224 (90%)	26 (10%)	9	25
1	E	250/259 (96%)	223 (89%)	27 (11%)	8	23
1	F	250/259 (96%)	227 (91%)	23 (9%)	11	32
All	All	1500/1554 (96%)	1345 (90%)	155 (10%)	9	26

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	216	ILE
1	D	99	LEU
1	F	163	ILE
1	C	235	LEU
1	C	314	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	286	GLN
1	D	231	GLN

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Mol	Chain	Res	Type
1	F	231	GLN
1	D	55	GLN
1	D	249	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.