



wwPDB X-ray Structure Validation Summary Report

May 22, 2020 – 11:27 am BST

PDB ID : 4DPL
Title : Structure of malonyl-coenzyme A reductase from crenarchaeota in complex with NadP
Authors : Demmer, U.; Warkentin, E.; Srivastava, A.; Kockelkorn, D.; Fuchs, G.; Ermler, U.
Deposited on : 2012-02-13
Resolution : 1.90 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 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) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

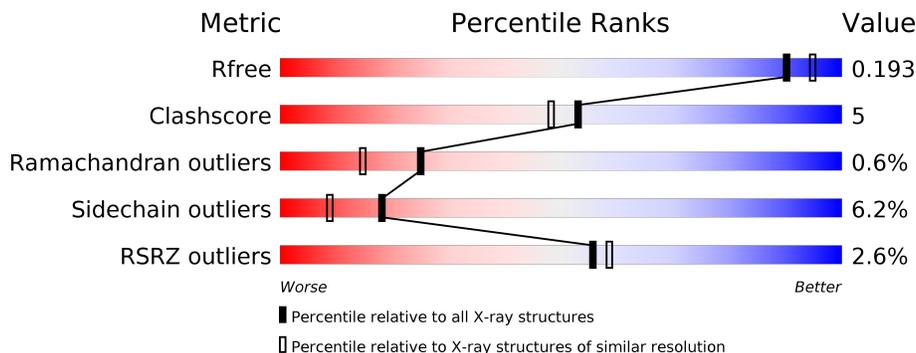
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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 $\leq 5\%$. 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	359	 2% 84% 13% ..
1	B	359	 % 86% 10% ..
1	C	359	 3% 85% 12% ..
1	D	359	 4% 84% 13% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNL	B	402	-	-	X	-
3	UNL	C	402	-	-	X	-

2 Entry composition [i](#)

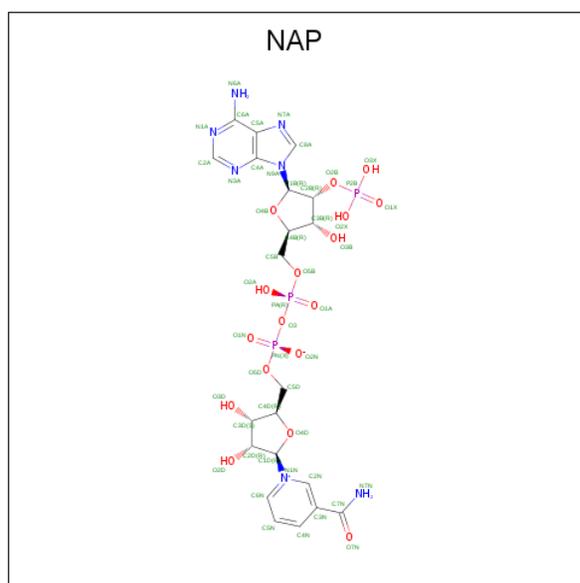
There are 4 unique types of molecules in this entry. The entry contains 12082 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Malonyl-CoA/succinyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	Total	C	N	O	S	0	1	0
			2746	1761	466	510	9			
1	B	354	Total	C	N	O	S	0	2	0
			2749	1763	466	511	9			
1	C	353	Total	C	N	O	S	0	1	0
			2738	1757	463	510	8			
1	D	354	Total	C	N	O	S	0	1	0
			2746	1761	466	510	9			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

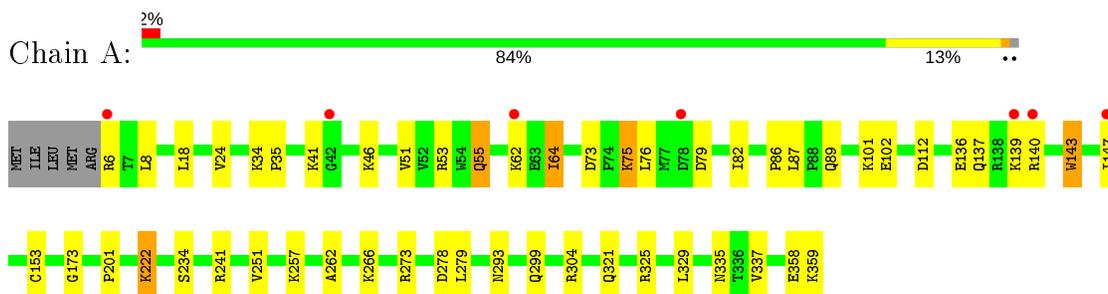
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	233	Total	O	0	0
			233	233		
4	B	225	Total	O	0	0
			225	225		
4	C	245	Total	O	0	0
			245	245		
4	D	184	Total	O	0	0
			184	184		

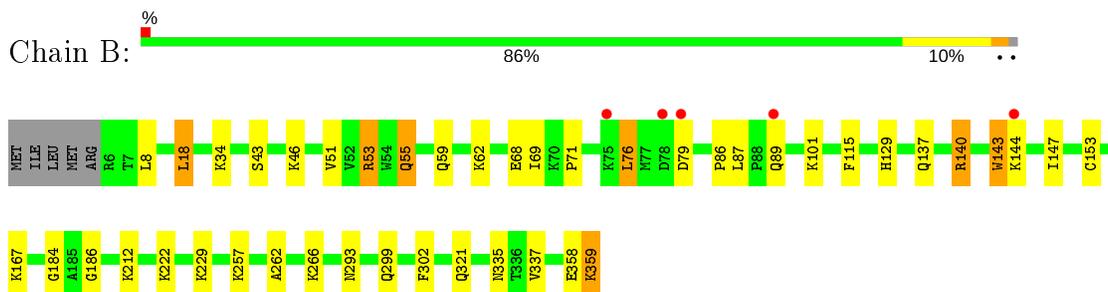
3 Residue-property plots [i](#)

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 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.

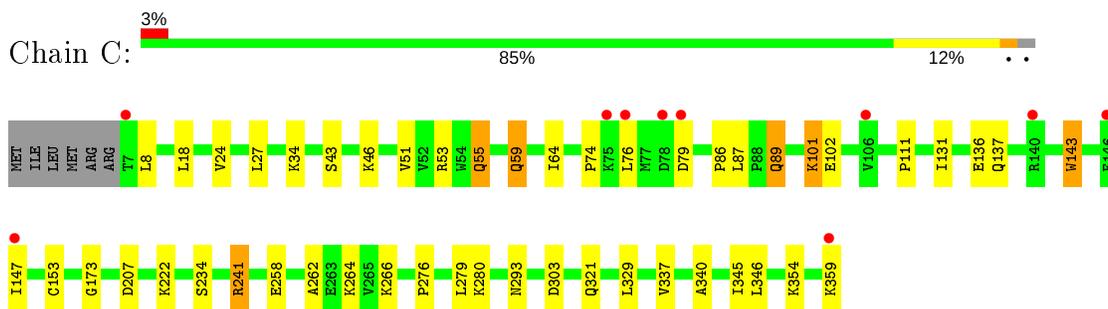
- Molecule 1: Malonyl-CoA/succinyl-CoA reductase



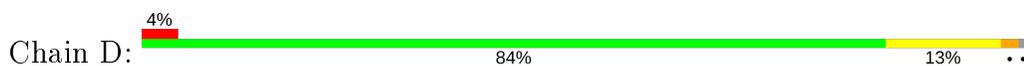
- Molecule 1: Malonyl-CoA/succinyl-CoA reductase

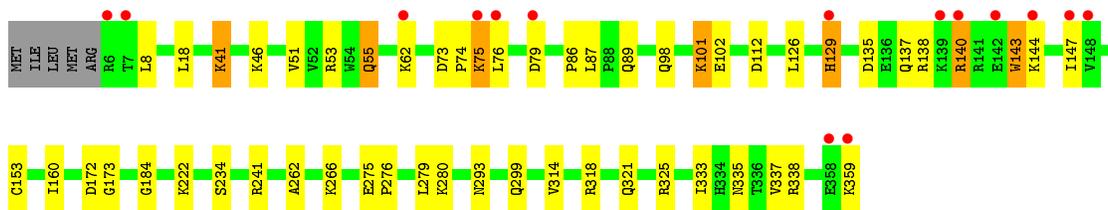


- Molecule 1: Malonyl-CoA/succinyl-CoA reductase



- Molecule 1: Malonyl-CoA/succinyl-CoA reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.58Å 128.80Å 140.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-1.90) 99.5 (19.95-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.6.0095	Depositor
R, R_{free}	0.163 , 0.194 0.162 , 0.193	Depositor DCC
R_{free} test set	6757 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12082	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 i

5.1 Standard geometry i

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

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	1.01	1/2810 (0.0%)	0.90	5/3816 (0.1%)
1	B	0.99	1/2816 (0.0%)	0.86	2/3824 (0.1%)
1	C	0.98	0/2802	0.89	5/3806 (0.1%)
1	D	0.93	3/2810 (0.1%)	0.85	5/3816 (0.1%)
All	All	0.98	5/11238 (0.0%)	0.87	17/15262 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	ARG	CZ-NH1	8.54	1.44	1.33
1	D	135	ASP	C-O	7.65	1.37	1.23
1	A	251	VAL	CB-CG2	5.78	1.65	1.52
1	D	314	VAL	CB-CG1	5.69	1.64	1.52
1	B	302	PHE	CE1-CZ	5.20	1.47	1.37

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	C	241	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	A	241	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	A	241	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	D	318	ARG	NE-CZ-NH1	7.31	123.95	120.30

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	2746	0	2803	29	0
1	B	2749	0	2808	29	0
1	C	2738	0	2793	33	0
1	D	2746	0	2803	29	0
2	A	48	0	25	0	0
2	B	48	0	25	3	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
3	A	6	0	0	1	0
3	B	6	0	0	2	0
3	C	6	0	0	3	0
3	D	6	0	0	1	0
4	A	233	0	0	2	0
4	B	225	0	0	1	0
4	C	245	0	0	5	0
4	D	184	0	0	3	0
All	All	12082	0	11307	120	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 5.

The worst 5 of 120 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:8:LEU:HD13	1:A:82:ILE:HD11	1.39	1.03
1:D:137:GLN:HE22	1:D:147:ILE:H	1.20	0.89
1:A:262:ALA:H	1:A:321:GLN:HE22	1.19	0.89
1:A:137:GLN:HE22	1:A:147:ILE:H	1.22	0.87
1:B:262:ALA:H	1:B:321:GLN:HE22	1.25	0.84

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	353/359 (98%)	344 (98%)	7 (2%)	2 (1%)	25	15
1	B	354/359 (99%)	343 (97%)	9 (2%)	2 (1%)	25	15
1	C	352/359 (98%)	341 (97%)	8 (2%)	3 (1%)	17	7
1	D	353/359 (98%)	340 (96%)	11 (3%)	2 (1%)	25	15
All	All	1412/1436 (98%)	1368 (97%)	35 (2%)	9 (1%)	25	15

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
1	B	86	PRO
1	C	86	PRO
1	D	86	PRO
1	C	340	ALA

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	298/302 (99%)	277 (93%)	21 (7%)	15	7
1	B	299/302 (99%)	278 (93%)	21 (7%)	15	7
1	C	297/302 (98%)	282 (95%)	15 (5%)	24	14
1	D	298/302 (99%)	280 (94%)	18 (6%)	19	9
All	All	1192/1208 (99%)	1117 (94%)	75 (6%)	18	8

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	140	ARG
1	B	359	LYS
1	D	140	ARG
1	B	143	TRP
1	B	229	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	293	ASN
1	C	129	HIS
1	D	293	ASN
1	B	321	GLN
1	C	55	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](#)

Of 8 ligands modelled in this entry, 4 are unknown - leaving 4 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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](#)

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	354/359 (98%)	-0.37	7 (1%) 65 68	16, 28, 59, 84	0
1	B	354/359 (98%)	-0.32	5 (1%) 75 77	15, 30, 58, 83	0
1	C	353/359 (98%)	-0.27	10 (2%) 53 56	16, 29, 58, 98	0
1	D	354/359 (98%)	-0.13	15 (4%) 36 39	17, 35, 67, 89	0
All	All	1415/1436 (98%)	-0.27	37 (2%) 56 58	15, 30, 62, 98	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	78	ASP	6.0
1	C	76	LEU	5.4
1	D	6	ARG	5.2
1	A	6	ARG	5.1
1	C	75	LYS	4.3

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 carbohydrates 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(\AA^2)	Q<0.9
2	NAP	B	401	48/48	0.84	0.25	30,62,84,103	0
3	UNL	B	402	6/-	0.88	0.14	36,40,41,43	0
3	UNL	D	402	6/-	0.89	0.15	33,40,48,50	0
3	UNL	A	402	6/-	0.90	0.11	31,35,41,44	0
3	UNL	C	402	6/-	0.90	0.14	33,37,43,59	0
2	NAP	A	401	48/48	0.91	0.17	31,52,63,69	0
2	NAP	D	401	48/48	0.92	0.18	35,59,73,90	0
2	NAP	C	401	48/48	0.93	0.14	29,45,56,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.