



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:23 AM GMT

PDB ID : 3EGO
Title : Crystal structure of Probable 2-dehydropantoate 2-reductase panE from Bacillus Subtilis
Authors : Ramagopal, U.A.; Toro, R.; Gilmore, M.; Hu, S.; Maletic, M.; Gheyi, T.; Bursley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-09-11
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
<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:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

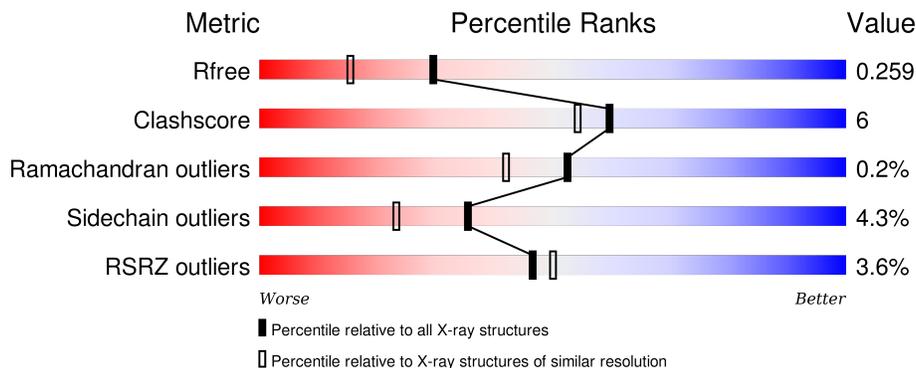
1 Overall quality at a glance

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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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. 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	307	 3% 80% 13% • 5%
1	B	307	 4% 82% 11% • 5%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 4798 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 Probable 2-dehydropantoate 2-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	292	Total	C	N	O	S	0	2	0
			2284	1457	391	427	9			
1	B	291	Total	C	N	O	S	0	5	0
			2312	1473	397	434	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP O34661
A	0	SER	-	expression tag	UNP O34661
A	1	LEU	-	expression tag	UNP O34661
A	298	GLU	-	expression tag	UNP O34661
A	299	GLY	-	expression tag	UNP O34661
A	300	HIS	-	expression tag	UNP O34661
A	301	HIS	-	expression tag	UNP O34661
A	302	HIS	-	expression tag	UNP O34661
A	303	HIS	-	expression tag	UNP O34661
A	304	HIS	-	expression tag	UNP O34661
A	305	HIS	-	expression tag	UNP O34661
B	-1	MET	-	expression tag	UNP O34661
B	0	SER	-	expression tag	UNP O34661
B	1	LEU	-	expression tag	UNP O34661
B	298	GLU	-	expression tag	UNP O34661
B	299	GLY	-	expression tag	UNP O34661
B	300	HIS	-	expression tag	UNP O34661
B	301	HIS	-	expression tag	UNP O34661
B	302	HIS	-	expression tag	UNP O34661
B	303	HIS	-	expression tag	UNP O34661
B	304	HIS	-	expression tag	UNP O34661
B	305	HIS	-	expression tag	UNP O34661

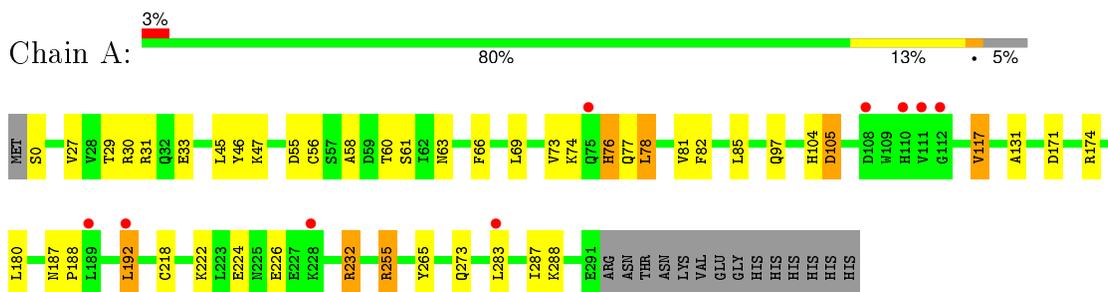
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	103	Total 103	O 103	0	0
2	B	99	Total 99	O 99	0	0

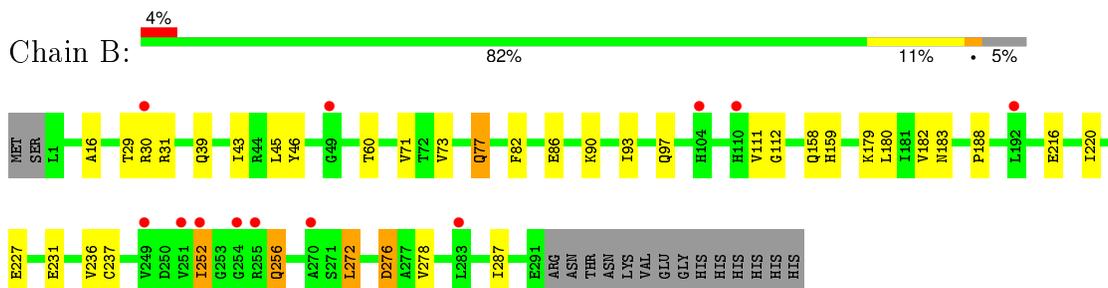
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

- Molecule 1: Probable 2-dehydropantoate 2-reductase



- Molecule 1: Probable 2-dehydropantoate 2-reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.86Å 43.66Å 83.76Å 90.00° 98.26° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 26.84 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-1.90) 99.6 (26.84-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.204 , 0.260 0.203 , 0.259	Depositor DCC
R_{free} test set	2319 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	31.4	Xtrriage
Anisotropy	0.506	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.8	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Outliers	1 of 45890 reflections (0.002%)	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4798	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.67	0/2333	0.72	2/3161 (0.1%)
1	B	0.63	0/2366	0.68	0/3203
All	All	0.65	0/4699	0.70	2/6364 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	VAL	CG1-CB-CG2	5.80	120.19	110.90
1	A	55	ASP	CB-CA-C	5.58	121.56	110.40

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	2284	0	2274	32	0
1	B	2312	0	2313	22	0
2	A	103	0	0	3	0
2	B	99	0	0	0	0
All	All	4798	0	4587	52	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 6.

All (52) 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:255:ARG:HD2	1:B:46:TYR:CE1	1.99	0.98
1:A:33:GLU:HG2	2:A:383:HOH:O	1.65	0.94
1:B:82:PHE:O	1:B:86:GLU:HG3	1.68	0.94
1:A:0:SER:HB2	2:A:384:HOH:O	1.85	0.77
1:A:76:HIS:HB2	2:A:376:HOH:O	1.84	0.77
1:A:61:SER:OG	1:A:63:ASN:ND2	2.21	0.73
1:B:30[A]:ARG:NH2	1:B:31:ARG:HE	1.91	0.68
1:B:30[A]:ARG:HH22	1:B:31:ARG:HE	1.49	0.59
1:B:73:VAL:HB	1:B:77[B]:GLN:HB2	1.86	0.58
1:A:232:ARG:CG	1:A:232:ARG:HH11	2.17	0.57
1:A:78:LEU:HG	1:A:82:PHE:CE2	2.41	0.55
1:A:187:ASN:HB2	1:A:188:PRO:HD3	1.89	0.54
1:A:255:ARG:HD2	1:B:46:TYR:CD1	2.40	0.54
1:B:276:ASP:OD2	1:B:278:VAL:HG23	2.09	0.53
1:B:90:LYS:CG	1:B:112:GLY:O	2.57	0.53
1:A:78:LEU:HD22	1:A:97:GLN:NE2	2.25	0.52
1:A:104:HIS:CE1	1:A:265:TYR:CD1	2.98	0.52
1:B:16:ALA:HB3	1:B:43:ILE:HD13	1.92	0.51
1:B:182:VAL:HG11	1:B:236:VAL:HG11	1.93	0.50
1:B:71:VAL:HG12	1:B:97:GLN:HE22	1.77	0.50
1:A:218:CYS:SG	1:A:226:GLU:HG2	2.53	0.49
1:A:171:ASP:OD2	1:A:174:ARG:HB2	2.13	0.48
1:A:81:VAL:O	1:A:85:LEU:HG	2.13	0.48
1:A:73:VAL:O	1:A:97:GLN:NE2	2.47	0.48
1:A:46:TYR:HE2	1:A:131:ALA:HB1	1.79	0.47
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.79	0.47
1:B:276:ASP:OD1	1:B:276:ASP:C	2.53	0.47
1:A:29:THR:O	1:A:60:THR:HA	2.14	0.47
1:B:252:ILE:HG13	1:B:252:ILE:H	1.49	0.46
1:B:158:GLN:HG2	1:B:159:HIS:CE1	2.51	0.46
1:B:188:PRO:HA	1:B:287:ILE:HD11	1.98	0.46
1:A:192:LEU:HD12	1:A:287:ILE:HD11	1.98	0.45
1:A:105:ASP:N	1:A:105:ASP:OD1	2.49	0.45
1:A:47:LYS:HE2	1:A:47:LYS:HB3	1.85	0.44
1:B:30[A]:ARG:NE	1:B:77[A]:GLN:OE1	2.45	0.44
1:A:232:ARG:CG	1:A:232:ARG:NH1	2.77	0.44
1:B:179:LYS:HE3	1:B:183:ASN:HD21	1.83	0.43
1:A:27:VAL:O	1:A:58:ALA:HA	2.19	0.42
1:A:66:PHE:CD2	1:A:69:LEU:HD21	2.54	0.42
1:B:272:LEU:HD23	1:B:272:LEU:N	2.33	0.42
1:A:283:LEU:O	1:A:287:ILE:HG12	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:HG3	1:A:31:ARG:HG3	2.02	0.42
1:A:78:LEU:HD22	1:A:97:GLN:HE21	1.83	0.42
1:B:256:GLN:HE21	1:B:256:GLN:HB2	1.65	0.41
1:B:29:THR:O	1:B:60:THR:HA	2.20	0.41
1:A:288:LYS:HA	1:A:288:LYS:HD2	1.96	0.41
1:A:222:LYS:HE3	1:A:273:GLN:OE1	2.21	0.41
1:B:216:GLU:O	1:B:220:ILE:HG13	2.20	0.41
1:B:227:GLU:O	1:B:231:GLU:HG2	2.21	0.40
1:A:76:HIS:CD2	1:A:76:HIS:H	2.33	0.40
1:A:74:LYS:HB3	1:A:76:HIS:CE1	2.57	0.40
1:A:27:VAL:HG23	1:A:56[A]:CYS:SG	2.61	0.40

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	292/307 (95%)	287 (98%)	4 (1%)	1 (0%)	46	35
1	B	294/307 (96%)	287 (98%)	7 (2%)	0	100	100
All	All	586/614 (95%)	574 (98%)	11 (2%)	1 (0%)	52	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	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	243/259 (94%)	233 (96%)	10 (4%)	37	25
1	B	247/259 (95%)	235 (95%)	12 (5%)	31	18
All	All	490/518 (95%)	468 (96%)	22 (4%)	35	21

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	76	HIS
1	A	77	GLN
1	A	78	LEU
1	A	105	ASP
1	A	117	VAL
1	A	180	LEU
1	A	192	LEU
1	A	232	ARG
1	A	255	ARG
1	B	39	GLN
1	B	45	LEU
1	B	77[A]	GLN
1	B	77[B]	GLN
1	B	93	ILE
1	B	111	VAL
1	B	180	LEU
1	B	237	CYS
1	B	252	ILE
1	B	256	GLN
1	B	272	LEU
1	B	276	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	76	HIS
1	A	215	GLN
1	A	239	GLN
1	B	79	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	159	HIS
1	B	160	ASN
1	B	183	ASN
1	B	239	GLN
1	B	256	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

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	292/307 (95%)	0.28	9 (3%) 52 56	20, 34, 56, 72	0
1	B	291/307 (94%)	0.30	12 (4%) 41 45	22, 33, 55, 64	0
All	All	583/614 (94%)	0.29	21 (3%) 46 50	20, 34, 56, 72	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	ILE	5.6
1	B	249	VAL	4.2
1	B	254	GLY	3.8
1	A	283	LEU	3.7
1	A	108	ASP	3.1
1	B	30[A]	ARG	3.0
1	B	192	LEU	3.0
1	B	255	ARG	2.9
1	A	112	GLY	2.9
1	A	110	HIS	2.8
1	A	189	LEU	2.7
1	B	49	GLY	2.5
1	A	192	LEU	2.5
1	B	283	LEU	2.5
1	B	270	ALA	2.4
1	B	110	HIS	2.4
1	B	251	VAL	2.4
1	A	75	GLN	2.3
1	B	104	HIS	2.2
1	A	111	VAL	2.2
1	A	228	LYS	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.