



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 30, 2021 – 03:51 PM EST

PDB ID : 3G17
Title : Structure of putative 2-dehydropantoate 2-reductase from staphylococcus aureus
Authors : Ramagopal, U.A.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-01-29
Resolution : 2.30 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
Xtriage (Phenix) : 1.13
EDS : 2.16
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) : 2.16

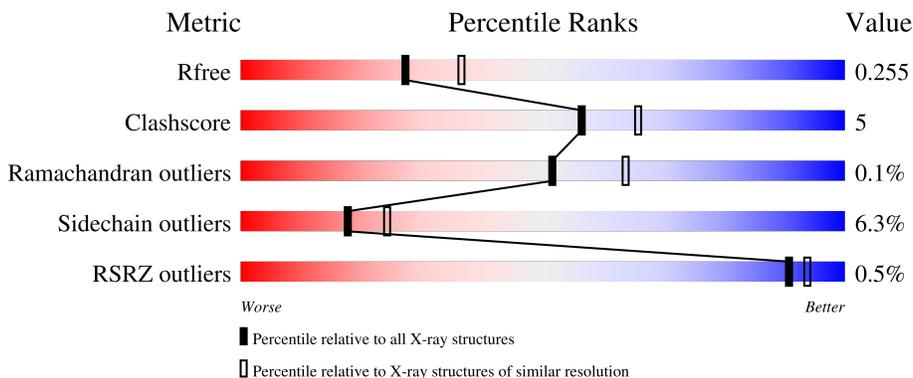
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	294	 85% 10% ..
1	B	294	 83% 13% ..
1	C	294	 80% 15% ..
1	D	294	 82% 14% ..
1	E	294	 86% 11% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	294	 <p>%</p> <p>73% 21% . .</p>
1	G	294	 <p>89% 9% ..</p>
1	H	294	 <p>86% 11% ..</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18687 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 Similar to 2-dehydropantoate 2-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	286	Total 2268	C 1449	N 389	O 423	S 7	0	0	0
1	B	286	Total 2278	C 1453	N 390	O 428	S 7	0	0	0
1	C	285	Total 2273	C 1452	N 388	O 426	S 7	0	1	0
1	D	287	Total 2291	C 1460	N 395	O 429	S 7	0	0	0
1	E	288	Total 2303	C 1467	N 399	O 430	S 7	0	1	0
1	F	282	Total 2245	C 1430	N 390	O 418	S 7	0	0	0
1	G	290	Total 2318	C 1477	N 403	O 431	S 7	0	0	0
1	H	290	Total 2315	C 1476	N 402	O 430	S 7	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q99R37
A	2	SER	-	expression tag	UNP Q99R37
A	287	GLU	-	expression tag	UNP Q99R37
A	288	GLY	-	expression tag	UNP Q99R37
A	289	HIS	-	expression tag	UNP Q99R37
A	290	HIS	-	expression tag	UNP Q99R37
A	291	HIS	-	expression tag	UNP Q99R37
A	292	HIS	-	expression tag	UNP Q99R37
A	293	HIS	-	expression tag	UNP Q99R37
A	294	HIS	-	expression tag	UNP Q99R37
B	1	MET	-	expression tag	UNP Q99R37
B	2	SER	-	expression tag	UNP Q99R37
B	287	GLU	-	expression tag	UNP Q99R37

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	288	GLY	-	expression tag	UNP Q99R37
B	289	HIS	-	expression tag	UNP Q99R37
B	290	HIS	-	expression tag	UNP Q99R37
B	291	HIS	-	expression tag	UNP Q99R37
B	292	HIS	-	expression tag	UNP Q99R37
B	293	HIS	-	expression tag	UNP Q99R37
B	294	HIS	-	expression tag	UNP Q99R37
C	1	MET	-	expression tag	UNP Q99R37
C	2	SER	-	expression tag	UNP Q99R37
C	287	GLU	-	expression tag	UNP Q99R37
C	288	GLY	-	expression tag	UNP Q99R37
C	289	HIS	-	expression tag	UNP Q99R37
C	290	HIS	-	expression tag	UNP Q99R37
C	291	HIS	-	expression tag	UNP Q99R37
C	292	HIS	-	expression tag	UNP Q99R37
C	293	HIS	-	expression tag	UNP Q99R37
C	294	HIS	-	expression tag	UNP Q99R37
D	1	MET	-	expression tag	UNP Q99R37
D	2	SER	-	expression tag	UNP Q99R37
D	287	GLU	-	expression tag	UNP Q99R37
D	288	GLY	-	expression tag	UNP Q99R37
D	289	HIS	-	expression tag	UNP Q99R37
D	290	HIS	-	expression tag	UNP Q99R37
D	291	HIS	-	expression tag	UNP Q99R37
D	292	HIS	-	expression tag	UNP Q99R37
D	293	HIS	-	expression tag	UNP Q99R37
D	294	HIS	-	expression tag	UNP Q99R37
E	1	MET	-	expression tag	UNP Q99R37
E	2	SER	-	expression tag	UNP Q99R37
E	287	GLU	-	expression tag	UNP Q99R37
E	288	GLY	-	expression tag	UNP Q99R37
E	289	HIS	-	expression tag	UNP Q99R37
E	290	HIS	-	expression tag	UNP Q99R37
E	291	HIS	-	expression tag	UNP Q99R37
E	292	HIS	-	expression tag	UNP Q99R37
E	293	HIS	-	expression tag	UNP Q99R37
E	294	HIS	-	expression tag	UNP Q99R37
F	1	MET	-	expression tag	UNP Q99R37
F	2	SER	-	expression tag	UNP Q99R37
F	287	GLU	-	expression tag	UNP Q99R37
F	288	GLY	-	expression tag	UNP Q99R37
F	289	HIS	-	expression tag	UNP Q99R37

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	290	HIS	-	expression tag	UNP Q99R37
F	291	HIS	-	expression tag	UNP Q99R37
F	292	HIS	-	expression tag	UNP Q99R37
F	293	HIS	-	expression tag	UNP Q99R37
F	294	HIS	-	expression tag	UNP Q99R37
G	1	MET	-	expression tag	UNP Q99R37
G	2	SER	-	expression tag	UNP Q99R37
G	287	GLU	-	expression tag	UNP Q99R37
G	288	GLY	-	expression tag	UNP Q99R37
G	289	HIS	-	expression tag	UNP Q99R37
G	290	HIS	-	expression tag	UNP Q99R37
G	291	HIS	-	expression tag	UNP Q99R37
G	292	HIS	-	expression tag	UNP Q99R37
G	293	HIS	-	expression tag	UNP Q99R37
G	294	HIS	-	expression tag	UNP Q99R37
H	1	MET	-	expression tag	UNP Q99R37
H	2	SER	-	expression tag	UNP Q99R37
H	287	GLU	-	expression tag	UNP Q99R37
H	288	GLY	-	expression tag	UNP Q99R37
H	289	HIS	-	expression tag	UNP Q99R37
H	290	HIS	-	expression tag	UNP Q99R37
H	291	HIS	-	expression tag	UNP Q99R37
H	292	HIS	-	expression tag	UNP Q99R37
H	293	HIS	-	expression tag	UNP Q99R37
H	294	HIS	-	expression tag	UNP Q99R37

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	74	Total O 74 74	0	0
2	B	60	Total O 60 60	0	0
2	C	51	Total O 51 51	0	0
2	D	38	Total O 38 38	0	0
2	E	31	Total O 31 31	0	0
2	F	29	Total O 29 29	0	0
2	G	60	Total O 60 60	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	53	Total	O	0	0
			53	53		



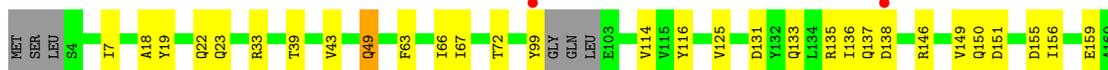
- Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain E: 86% 11% ..



- Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain F: % 73% 21% ..



- Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain G: 89% 9% ..



- Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain H: 86% 11% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.24Å 99.64Å 100.26Å 103.66° 105.23° 102.26°	Depositor
Resolution (Å)	50.00 – 2.30 37.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.30) 98.2 (37.55-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.29Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.260 0.198 , 0.255	Depositor DCC
R_{free} test set	5744 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.007 for -h,-l,-k	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18687	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 5.21% 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 [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	0.61	0/2314	0.68	0/3155
1	B	0.63	0/2324	0.67	0/3168
1	C	0.56	0/2322	0.65	0/3166
1	D	0.63	0/2339	0.69	0/3188
1	E	0.62	0/2355	0.66	0/3210
1	F	0.54	0/2291	0.65	0/3121
1	G	0.63	1/2368 (0.0%)	0.70	1/3228 (0.0%)
1	H	0.58	0/2365	0.66	0/3224
All	All	0.60	1/18678 (0.0%)	0.67	1/25460 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	111	CYS	CB-SG	-5.72	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	226	MET	CA-CB-CG	-5.34	104.22	113.30

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	2268	0	2254	23	0
1	B	2278	0	2264	20	0
1	C	2273	0	2259	33	0
1	D	2291	0	2269	22	0
1	E	2303	0	2281	20	0
1	F	2245	0	2218	40	0
1	G	2318	0	2294	14	0
1	H	2315	0	2290	25	0
2	A	74	0	0	2	0
2	B	60	0	0	0	0
2	C	51	0	0	0	0
2	D	38	0	0	0	0
2	E	31	0	0	0	0
2	F	29	0	0	1	0
2	G	60	0	0	0	0
2	H	53	0	0	0	0
All	All	18687	0	18129	182	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 182 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:B:262:ARG:HH11	1:B:262:ARG:HG3	1.19	1.01
1:H:137:GLN:O	1:H:142:THR:HG21	1.68	0.91
1:F:137:GLN:HE21	1:F:138:ASP:H	1.16	0.89
1:B:262:ARG:NH1	1:B:262:ARG:HG3	1.85	0.88
1:F:171:LEU:HD11	1:F:206:GLY:HA3	1.56	0.86

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	284/294 (97%)	273 (96%)	11 (4%)	0	100	100
1	B	284/294 (97%)	269 (95%)	15 (5%)	0	100	100
1	C	284/294 (97%)	270 (95%)	14 (5%)	0	100	100
1	D	285/294 (97%)	275 (96%)	10 (4%)	0	100	100
1	E	287/294 (98%)	276 (96%)	11 (4%)	0	100	100
1	F	276/294 (94%)	255 (92%)	19 (7%)	2 (1%)	22	26
1	G	288/294 (98%)	278 (96%)	10 (4%)	0	100	100
1	H	288/294 (98%)	276 (96%)	12 (4%)	0	100	100
All	All	2276/2352 (97%)	2172 (95%)	102 (4%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	188	ALA
1	F	255	ILE

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	244/256 (95%)	230 (94%)	14 (6%)	20	28
1	B	247/256 (96%)	227 (92%)	20 (8%)	11	15
1	C	246/256 (96%)	227 (92%)	19 (8%)	13	16
1	D	248/256 (97%)	230 (93%)	18 (7%)	14	18
1	E	250/256 (98%)	239 (96%)	11 (4%)	28	39
1	F	242/256 (94%)	220 (91%)	22 (9%)	9	11
1	G	251/256 (98%)	243 (97%)	8 (3%)	39	54
1	H	250/256 (98%)	237 (95%)	13 (5%)	23	32
All	All	1978/2048 (97%)	1853 (94%)	125 (6%)	18	24

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	71	LYS
1	D	275	THR
1	H	71	LYS
1	D	89	ASP
1	D	179	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	164	GLN
1	F	137	GLN
1	H	177	ASN
1	F	96	GLN
1	F	144	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 monosaccharides 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](#)

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	286/294 (97%)	-0.36	2 (0%) 87 91	22, 32, 47, 53	0
1	B	286/294 (97%)	-0.21	2 (0%) 87 91	22, 36, 59, 64	0
1	C	285/294 (96%)	-0.22	1 (0%) 92 95	25, 39, 54, 61	0
1	D	287/294 (97%)	-0.30	0 100 100	20, 33, 51, 60	0
1	E	288/294 (97%)	-0.41	0 100 100	20, 33, 48, 62	0
1	F	282/294 (95%)	-0.04	4 (1%) 75 80	27, 44, 63, 66	0
1	G	290/294 (98%)	-0.39	1 (0%) 94 96	20, 31, 45, 59	0
1	H	290/294 (98%)	-0.40	1 (0%) 94 96	23, 35, 48, 57	0
All	All	2294/2352 (97%)	-0.29	11 (0%) 91 94	20, 35, 56, 66	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	GLY	2.9
1	F	218	SER	2.9
1	B	216	ASN	2.7
1	G	292	HIS	2.6
1	A	84	TYR	2.5

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.