



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:35 AM GMT

PDB ID : 3BAN
Title : The crystal structure of mannonate dehydratase from Streptococcus suis serotype2
Authors : Peng, H.; Zhang, Q.M.; Gao, F.; Liu, Y.W.; Qi, J.X.; Gao, G.F.
Deposited on : 2007-11-08
Resolution : 2.90 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
<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

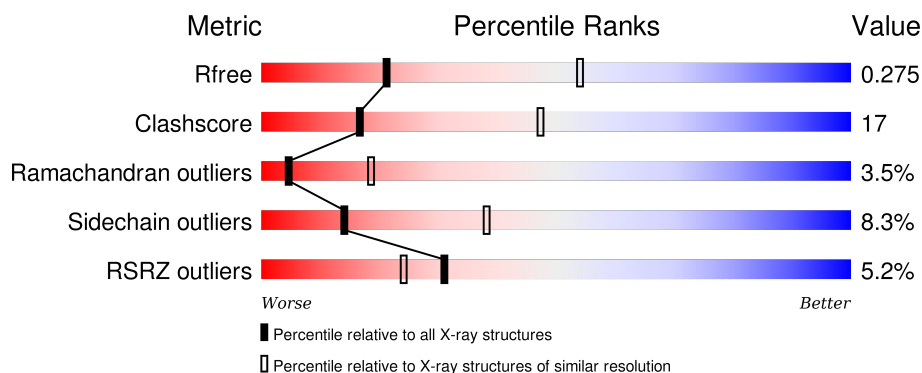
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	386	<div> <div>4%</div> <div>56%</div> <div>28%</div> <div>6%</div> <div>10%</div> </div>
1	B	386	<div> <div>5%</div> <div>59%</div> <div>28%</div> <div>•</div> <div>10%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5471 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 D-mannonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2738	1745	465	514	14			
1	B	349	Total	C	N	O	S	0	0	0
			2733	1742	465	513	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP A4VVI4
A	2	GLY	-	EXPRESSION TAG	UNP A4VVI4
A	3	SER	-	EXPRESSION TAG	UNP A4VVI4
A	4	SER	-	EXPRESSION TAG	UNP A4VVI4
A	5	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	6	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	7	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	8	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	9	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	10	HIS	-	EXPRESSION TAG	UNP A4VVI4
A	11	SER	-	EXPRESSION TAG	UNP A4VVI4
A	12	SER	-	EXPRESSION TAG	UNP A4VVI4
A	13	GLY	-	EXPRESSION TAG	UNP A4VVI4
A	14	LEU	-	EXPRESSION TAG	UNP A4VVI4
A	15	VAL	-	EXPRESSION TAG	UNP A4VVI4
A	16	PRO	-	EXPRESSION TAG	UNP A4VVI4
A	17	ARG	-	EXPRESSION TAG	UNP A4VVI4
A	18	GLY	-	EXPRESSION TAG	UNP A4VVI4
A	19	SER	-	EXPRESSION TAG	UNP A4VVI4
A	20	HIS	-	EXPRESSION TAG	UNP A4VVI4
B	1	MET	-	EXPRESSION TAG	UNP A4VVI4
B	2	GLY	-	EXPRESSION TAG	UNP A4VVI4
B	3	SER	-	EXPRESSION TAG	UNP A4VVI4
B	4	SER	-	EXPRESSION TAG	UNP A4VVI4
B	5	HIS	-	EXPRESSION TAG	UNP A4VVI4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	EXPRESSION TAG	UNP A4VVI4
B	7	HIS	-	EXPRESSION TAG	UNP A4VVI4
B	8	HIS	-	EXPRESSION TAG	UNP A4VVI4
B	9	HIS	-	EXPRESSION TAG	UNP A4VVI4
B	10	HIS	-	EXPRESSION TAG	UNP A4VVI4
B	11	SER	-	EXPRESSION TAG	UNP A4VVI4
B	12	SER	-	EXPRESSION TAG	UNP A4VVI4
B	13	GLY	-	EXPRESSION TAG	UNP A4VVI4
B	14	LEU	-	EXPRESSION TAG	UNP A4VVI4
B	15	VAL	-	EXPRESSION TAG	UNP A4VVI4
B	16	PRO	-	EXPRESSION TAG	UNP A4VVI4
B	17	ARG	-	EXPRESSION TAG	UNP A4VVI4
B	18	GLY	-	EXPRESSION TAG	UNP A4VVI4
B	19	SER	-	EXPRESSION TAG	UNP A4VVI4
B	20	HIS	-	EXPRESSION TAG	UNP A4VVI4

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 ($\text{RSRZ} > 2$). 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.

Chain A:

4% 56% 28% 6% 10%

MET GLY SER SER HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY S19 H20 K21 K22 W23 S24 F25 R26 D32 P33 V34 L36 G44 I48 V49 F50 A51 Y52 Y53 D54 V55 P56 W57 G58 G59 A60 A61 P62 L63 E64 N65 T66 L67 L69 W73 V74 E75 T81 V82 I83 E84 S85 I86 I92 K96 P97 N98 L102 T103 E104 Y106 K107 T108 S109 I110 R111 N112 A116 G117 T118 P119 V120 V121 C122 Y123 I124 F125 M126 D130 H137 P141 G142 L154 P159 VAL ALA ASP ASP LEU ASN LEU PRO GLY TRP ASD SER SER TTR S174 E175 E177 I181 S190 D193 S194 W195 L198 E199 L206 P207 T208 A209 E210 E211 H219 P220 G226 P231 R232 E238 R242 F243 L244 N245 L246 Y247 D248 S249 E250 H251 N252 Y256 C257 Y261 V266 L270 N280 R281 H286 T287 R288 T291 A292 G293 W295 E299 I303 S304 Q305 D308 P311 N312 A313 V314 V315 V319 D320 V321 D322 S326 L327 R328 P329 D330 H331 R334 I335 V336 W337 P343 G344 G346 G347 L347 V348 D349 R350 A351 L352 G353 A354 T355 Y356 F357 A363 I364 R365 D366

Chain B:

5% 59% 28% 10%

ASN
LEU
PRO
GLY
TRP
SER
SER
TYR
SER
LYS
GLU
GLU
MET
LYS
I180
I181
I182
E183
N184
Y185
R186
Q187
N188
E189
I202
K215
E219
P220
D221
D222
Y225
G226
I227
F228
Q229
R232
G236
V240
E241
R242
F243
L244
N245
L246
I254
Y261
A262
S263
D264

P285
K286
N287
E274
Y275
K278
R279
M280
N283
F284
M285
E286
F287
Q288
N289
A292
G293
F297
L303
S304
I309
N312
L327
R328
P329
D330
E331
R334
I335
D338
Q339
T340
K341
F342
P343
G344
A351
L352
G353
A354
T355
Y356
F357
N358
Y361
F362
L363

I364	I365	I366	I367	T371	A378	T383	K384	E385	GLY
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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.69 Å 105.69 Å 159.57 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.06 – 2.90 44.06 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.06-2.90) 99.8 (44.06-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.44 (at 2.90 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.286 0.230 , 0.275	Depositor DCC
R_{free} test set	1063 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	51.9	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 20698 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5471	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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, 0.375 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	0.68	2/2805 (0.1%)	0.77	0/3808
1	B	0.68	0/2800	0.81	0/3802
All	All	0.68	2/5605 (0.0%)	0.79	0/7610

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	GLU	CG-CD	6.01	1.60	1.51
1	A	250	GLU	CB-CG	5.46	1.62	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	SER	Peptide

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	2738	0	2676	100	0
1	B	2733	0	2679	83	0
All	All	5471	0	5355	179	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 17.

The worst 5 of 179 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:250:GLU:HG2	1:A:280:ASN:HD22	1.16	1.06
1:B:199:GLU:HB2	1:B:246:LEU:CD2	1.92	0.98
1:B:182:ILE:HG22	1:B:186:ARG:HD2	1.49	0.94
1:A:57:VAL:HG13	1:A:58:GLY:H	1.37	0.90
1:B:61:TRP:O	1:B:112:ASN:ND2	2.06	0.88

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	345/386 (89%)	295 (86%)	40 (12%)	10 (3%)	6	23
1	B	345/386 (89%)	290 (84%)	41 (12%)	14 (4%)	3	14
All	All	690/772 (89%)	585 (85%)	81 (12%)	24 (4%)	4	18

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	A	116	ALA
1	A	343	PRO

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Mol	Chain	Res	Type
1	B	97	PRO
1	B	128	VAL

5.3.2 Protein sidechains ⓘ

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	288/321 (90%)	260 (90%)	28 (10%)	10	30
1	B	288/321 (90%)	268 (93%)	20 (7%)	19	48
All	All	576/642 (90%)	528 (92%)	48 (8%)	14	38

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	GLN
1	A	350	ARG
1	B	341	LYS
1	A	315	VAL
1	A	330	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	GLN
1	A	358	ASN
1	B	286	HIS
1	A	298	GLN
1	A	312	ASN

5.3.3 RNA ⓘ

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](#)

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	349/386 (90%)	0.17	17 (4%) 33 27	21, 42, 62, 69	0
1	B	349/386 (90%)	0.14	19 (5%) 29 23	19, 38, 64, 82	0
All	All	698/772 (90%)	0.15	36 (5%) 31 24	19, 40, 62, 82	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	GLY	9.9
1	B	339	GLN	4.1
1	B	187	GLN	3.9
1	B	138	HIS	3.8
1	A	60	ALA	3.7

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.