



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:18 AM GMT

PDB ID : 3LN7  
Title : Crystal structure of a bifunctional glutathione synthetase from *Pasteurella multocida*  
Authors : Stout, J.; Vergauwen, B.; Savvides, S.N.  
Deposited on : 2010-02-02  
Resolution : 3.20 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](mailto: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.

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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

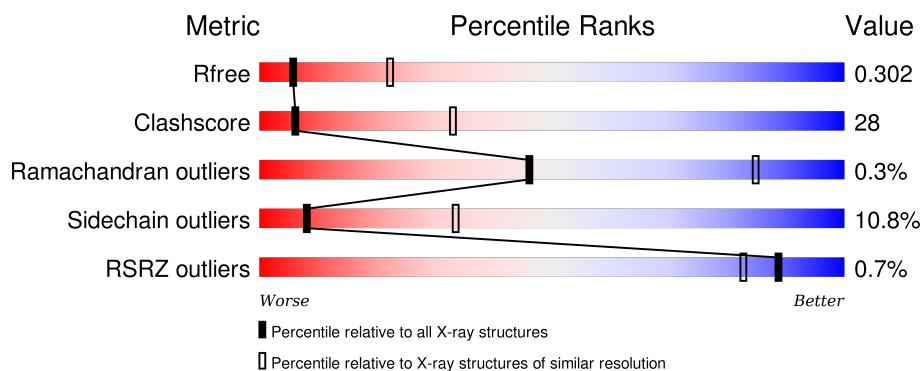
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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  $\geq 3$ , 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	757	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>38%</div> <div>• •</div> </div> </div>
1	B	757	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>37%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10601 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.

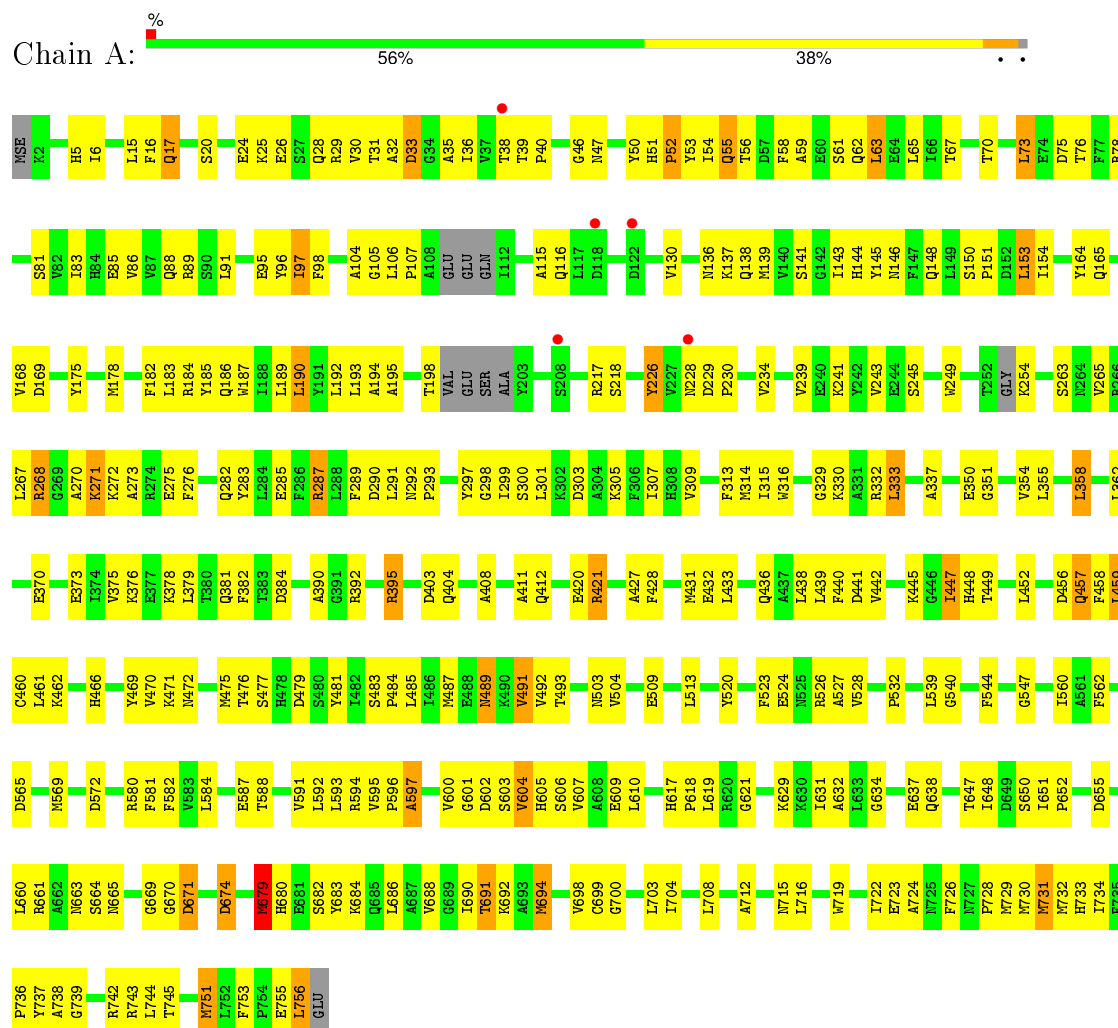
- Molecule 1 is a protein called Glutathione biosynthesis bifunctional protein gshAB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	Se	0	1	0
			5402	3467	912	1003	2	18			
1	B	729	Total	C	N	O	S	Se	0	0	0
			5199	3329	871	980	2	17			

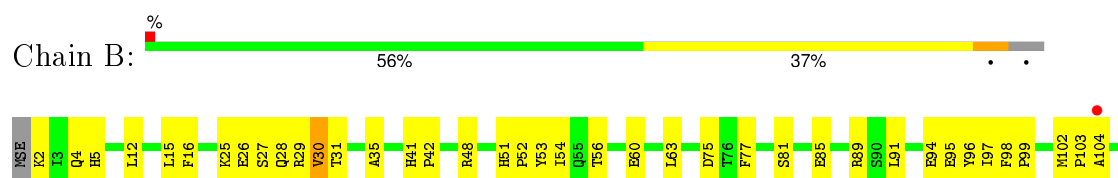
### 3 Residue-property plots

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

- Molecule 1: Glutathione biosynthesis bifunctional protein gshAB



- Molecule 1: Glutathione biosynthesis bifunctional protein gshAB



E723	E724	N725	F726	N727	P728	N729	N730	N731	N732	N733	I734	F735	F736	Y737	A738	L744	T745	L752	F753	P754	E755	L756	GLU	D453	Q545	I636	K361	R268	T196	V114																					
E637	G547	L639	N640	L641	Q644	G645	L646	T647	I648	D649	S650	I651	P652	D655	Q656	L657	V658	Q659	L660	R661	A662	N663	S664	N665	D671	S672	M679	H680	E681	S682	Y683	L686	I690	T691	M694	A697	V698	C699	L703	I704	I705	P706	D707	L708	A712	S718	W719				
Q546	G548	N550	D553	F554	A557	L558	E559	I560	F562	S563	E564	Y573	H580	F581	F582	V583	L584	G585	D586	E587	L592	V595	P596	V600	G601	D602	S603	V604	H605	S606	V607	L610	W611	A612	D616	H617	F618	L619	H620	G621	P627	L628	H629	B635							
D456	Q457	F458	L459	C460	L461	K462	Y463	V470	K471	N472	G473	N474	M475	T476	Y481	S483	P484	L485	L486	M487	E488	N489	K490	V491	V492	T493	L497	A500	L513	E514	K515	Y520	F523	GLU	ASN	R526	V529	I530	K531	P532	K533	G538	L539	G540	I541	T542					
A273	R274	E275	F276	Y283	L284	E285	D286	R287	L288	F289	D290	N292	P293	F294	Y297	L301	F310	A311	L312	F313	N314	I315	K316	N317	D318	H319	THR	ALA	D322	Q323	V326	L333	A334	E335	V336	A337	P341	T345	A348	V349	E350	V354	E357	S360							
L362	I365	G366	A367	F372	E377	K378	I381	F382	T383	P385	T388	V389	A390	V394	I397	E398	Q404	Q405	Q409	L410	A411	Q412	K415	A416	F419	Y423	A427	P428	D429	M430	M431	E432	L433	Q436	L439	I447	H448	T449	E450	I451	L452										
P197	T198	Y199	E200	S201	ALA	TYR	F204	K205	D206	G207	S208	PRO	LEU	V130	ALA	LYS	P293	F294	R217	S218	L219	S220	S221	Y226	Y227	N228	ASP	P230	V234	S235	S238	V239	E240	K241	V242	V243	E244	N172	D173	L174	Y175	L176	K177	M178	F182	Q186	W187	I188	L189	L192	A195

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	205.24Å 87.07Å 145.98Å 90.00° 126.53° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 19.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-3.20) 97.1 (19.90-3.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 3.22Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.275 , 0.314 0.269 , 0.302	Depositor DCC
$R_{free}$ test set	1669 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.7	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 45.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 33404 reflections	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	10601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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	0/5491	0.74	4/7456 (0.1%)
1	B	0.63	0/5280	0.73	4/7177 (0.1%)
All	All	0.65	0/10771	0.74	8/14633 (0.1%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	679	MSE	CG-SE-CE	6.12	112.36	98.90
1	A	491	VAL	CB-CA-C	-5.89	100.20	111.40
1	B	220	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	332	ARG	CG-CD-NE	5.72	123.80	111.80
1	A	332	ARG	NE-CZ-NH1	-5.17	117.71	120.30

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	5402	0	4799	290	0
1	B	5199	0	4516	280	0
All	All	10601	0	9315	562	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 28.

The worst 5 of 562 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:679:MSE:HE3	1:A:708:LEU:HD23	1.46	0.97
1:A:647:THR:H	1:A:650:SER:HB3	1.31	0.93
1:A:730:MSE:HE3	1:A:745:THR:HG22	1.51	0.93
1:A:30:VAL:HG22	1:A:36:ILE:HA	1.57	0.85
1:B:238:SER:HB3	1:B:241:LYS:HB2	1.58	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	740/757 (98%)	713 (96%)	23 (3%)	4 (0%)	34	78
1	B	713/757 (94%)	690 (97%)	22 (3%)	1 (0%)	56	91
All	All	1453/1514 (96%)	1403 (97%)	45 (3%)	5 (0%)	46	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	604	VAL
1	B	548	VAL
1	A	457	GLN
1	A	52	PRO
1	A	597	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	462/637 (72%)	415 (90%)	47 (10%)	9	36
1	B	435/637 (68%)	385 (88%)	50 (12%)	7	30
All	All	897/1274 (70%)	800 (89%)	97 (11%)	8	33

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	715	ASN
1	B	139	MSE
1	B	610	LEU
1	A	751	MSE
1	B	27	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	466	HIS
1	A	733	HIS
1	B	605	HIS
1	A	663	ASN
1	A	665	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	728/757 (96%)	-0.37	5 (0%) 89 83	20, 39, 66, 88	0
1	B	710/757 (93%)	-0.36	5 (0%) 89 83	20, 41, 71, 102	0
All	All	1438/1514 (94%)	-0.37	10 (0%) 89 83	20, 40, 68, 102	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	SER	3.4
1	B	208	SER	3.4
1	B	104	ALA	3.0
1	A	228	ASN	2.6
1	B	226	TYR	2.6

### 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.