



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:00 PM GMT

PDB ID : 1K3O  
Title : Crystal Structure Analysis of apo Glutathione S-Transferase  
Authors : Le Trong, I.; Stenkamp, R.E.; Ibarra, C.; Atkins, W.M.; Adman, E.T.  
Deposited on : 2001-10-03  
Resolution : 1.80 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

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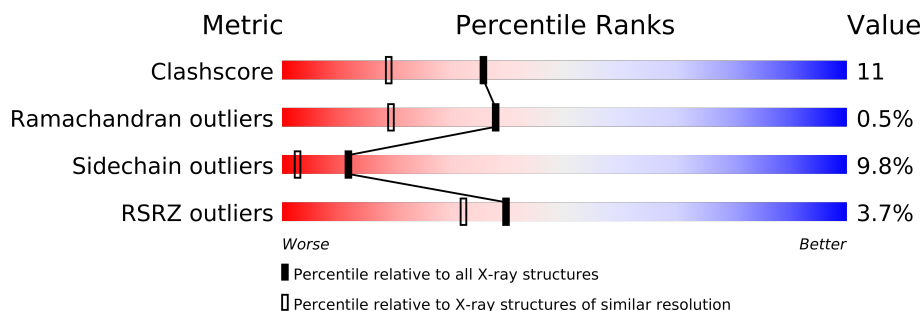
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	221	
1	B	221	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3544 atoms, of which 0 are hydrogen and 0 are deuterium.

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 S-TRANSFERASE A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	2	1	0
			1610	1046	270	287	7			
1	B	208	Total	C	N	O	S	22	2	0
			1687	1094	282	303	8			

- Molecule 2 is water.

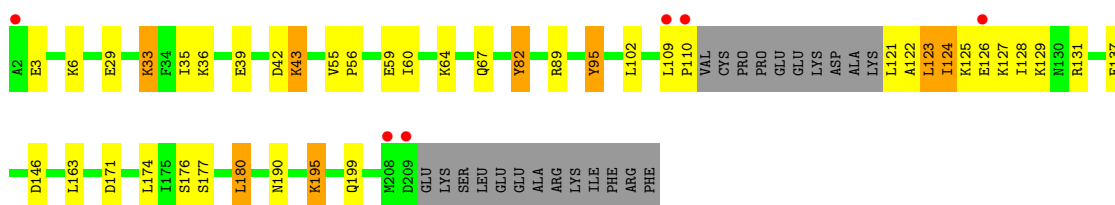
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		
2	B	133	Total	O	0	0
			133	133		

### 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 ( $RSRZ > 2$ ). 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.

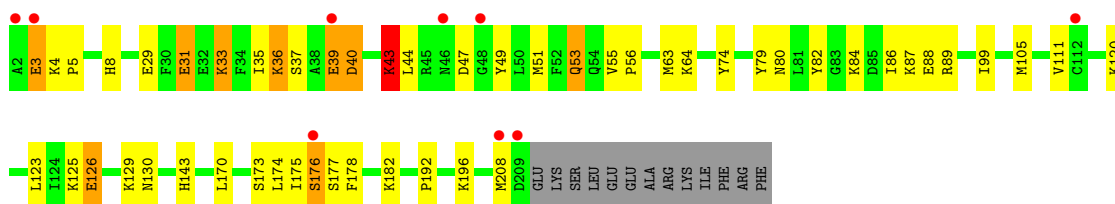
- Molecule 1: GLUTATHIONE S-TRANSFERASE A1

Chain A:



- Molecule 1: GLUTATHIONE S-TRANSFERASE A1

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.38Å 96.01Å 52.89Å 90.00° 92.94° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 10.00 – 1.79	Depositor EDS
% Data completeness (in resolution range)	90.8 (10.00-1.80) 84.6 (10.00-1.79)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 1.79Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.246 , 0.336 0.221 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 118.9	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43467 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3544	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 7.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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	0.35	0/1645	1.01	3/2211 (0.1%)
1	B	0.59	2/1732 (0.1%)	1.01	2/2330 (0.1%)
All	All	0.49	2/3377 (0.1%)	1.01	5/4541 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	LYS	CE-NZ	-18.83	1.01	1.49
1	B	43	LYS	CE-NZ	6.59	1.65	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	TYR	CB-CG-CD1	7.01	125.20	121.00
1	A	95	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	B	74	TYR	CB-CG-CD2	5.64	124.39	121.00
1	B	99	ILE	O-C-N	-5.62	113.71	122.70
1	A	146	ASP	CB-CG-OD1	5.05	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1610	0	1673	32	0
1	B	1687	0	1746	40	0
2	A	114	0	0	4	0
2	B	133	0	0	4	0
All	All	3544	0	3419	70	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (70) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:125:LYS:O	1:B:129:LYS:HG2	1.59	1.02
1:A:121:LEU:HA	1:A:124:ILE:HG13	1.56	0.86
1:A:124:ILE:O	1:A:128:ILE:HG13	1.83	0.78
1:B:126:GLU:HA	1:B:129:LYS:HE2	1.66	0.77
1:A:137:GLU:OE2	1:A:180:LEU:HG	1.87	0.75
1:A:125:LYS:O	1:A:129:LYS:HE2	1.89	0.73
1:A:125:LYS:O	1:A:129:LYS:HG3	1.90	0.72
1:B:8:HIS:ND1	1:B:33:LYS:HD2	2.04	0.71
1:B:192:PRO:O	1:B:196:LYS:HG3	1.93	0.69
1:A:180:LEU:HD21	2:A:6106:HOH:O	1.93	0.68
1:B:86:ILE:HG22	1:B:89[B]:ARG:NH2	2.08	0.67
1:A:109:LEU:HD21	1:A:121:LEU:HD13	1.76	0.66
1:B:4:LYS:HD2	1:B:31:GLU:HG2	1.78	0.66
1:A:127:LYS:HD2	1:A:131:ARG:NH1	2.11	0.65
1:B:89[A]:ARG:HD3	2:B:6194:HOH:O	1.98	0.64
1:A:33:LYS:O	1:A:33:LYS:HG3	1.98	0.64
1:B:126:GLU:HG2	1:B:129:LYS:HE2	1.79	0.63
1:B:129:LYS:HE3	1:B:130:ASN:HD21	1.65	0.61
1:B:84:LYS:HG2	1:B:88:GLU:OE1	2.01	0.60
1:B:208:MET:HB2	2:B:6234:HOH:O	2.01	0.59
1:A:195:LYS:HD2	2:A:6310:HOH:O	2.03	0.58
1:B:33:LYS:HE3	1:B:35:ILE:HG13	1.84	0.58
1:B:39:GLU:HG2	1:B:40:ASP:N	2.18	0.58
1:A:89[B]:ARG:HD3	2:B:6095:HOH:O	2.04	0.57
1:A:109:LEU:HD21	1:A:121:LEU:CD1	2.34	0.57
1:B:86:ILE:HG22	1:B:89[B]:ARG:HH22	1.67	0.57
1:B:129:LYS:HE3	1:B:130:ASN:ND2	2.18	0.57
1:A:127:LYS:HD2	1:A:131:ARG:HH11	1.68	0.57
1:A:102:LEU:HD23	1:A:163:LEU:HD21	1.87	0.57
1:B:126:GLU:HA	1:B:129:LYS:CE	2.35	0.56
1:B:33:LYS:O	1:B:33:LYS:HD3	2.06	0.55
1:B:33:LYS:HE2	1:B:44:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:33:LYS:HE3	1:B:35:ILE:CG1	2.39	0.53
1:B:63:MET:C	1:B:64:LYS:HD2	2.30	0.52
1:B:126:GLU:O	1:B:129:LYS:HG3	2.10	0.52
1:A:122:ALA:O	1:A:126:GLU:HG3	2.08	0.51
1:A:82:TYR:CE1	1:A:89[B]:ARG:HG3	2.46	0.50
1:B:37:SER:OG	1:B:39:GLU:OE1	2.30	0.50
1:B:4:LYS:HD2	1:B:31:GLU:CG	2.40	0.50
1:B:87:LYS:HG3	2:B:6249:HOH:O	2.11	0.49
1:B:47:ASP:HB3	1:B:49:TYR:CE1	2.48	0.49
1:A:171:ASP:HB3	1:A:174:LEU:HD12	1.95	0.49
1:A:6:LYS:HE2	1:A:59:GLU:OE2	2.13	0.49
1:B:55:VAL:HB	1:B:56:PRO:HA	1.95	0.48
1:A:171:ASP:HB3	1:A:174:LEU:CD1	2.43	0.48
1:B:173:SER:O	1:B:176:SER:OG	2.30	0.47
1:A:95:TYR:HE1	1:B:51[A]:MET:HE1	1.80	0.47
1:B:84:LYS:HE3	1:B:88:GLU:OE2	2.15	0.46
1:B:79:TYR:O	1:B:80:ASN:HB2	2.15	0.46
1:A:43:LYS:HB3	1:A:43:LYS:HE3	1.32	0.45
1:B:43:LYS:O	1:B:47:ASP:HB2	2.16	0.45
1:A:55:VAL:HB	1:A:56:PRO:HA	1.98	0.45
1:B:126:GLU:OE2	1:B:130:ASN:ND2	2.50	0.45
1:A:137:GLU:CD	1:A:180:LEU:HG	2.37	0.45
1:B:37:SER:OG	1:B:40:ASP:OD1	2.30	0.44
1:A:125:LYS:C	1:A:129:LYS:HE2	2.37	0.44
1:A:199:GLN:NE2	2:A:6228:HOH:O	2.49	0.44
1:A:33:LYS:HG3	2:A:6250:HOH:O	2.18	0.43
1:B:84:LYS:HG2	1:B:88:GLU:CD	2.38	0.43
1:B:47:ASP:HB3	1:B:49:TYR:HE1	1.82	0.43
1:B:125:LYS:HB3	1:B:174:LEU:HD21	2.00	0.42
1:A:131:ARG:HH21	1:B:53:GLN:HB2	1.86	0.41
1:A:109:LEU:HB3	1:A:110:PRO:HD3	2.03	0.41
1:A:123:LEU:HA	1:A:123:LEU:HD13	1.79	0.41
1:A:121:LEU:O	1:A:125:LYS:N	2.53	0.41
1:B:4:LYS:HA	1:B:5:PRO:HD3	1.96	0.41
1:A:35:ILE:HG21	1:A:35:ILE:HD13	1.86	0.41
1:B:175:ILE:HG12	1:B:175:ILE:O	2.21	0.40
1:B:178:PHE:O	1:B:182:LYS:HG3	2.21	0.40
1:A:60:ILE:HD13	1:A:60:ILE:HG21	1.90	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	195/221 (88%)	189 (97%)	5 (3%)	1 (0%)	38	19
1	B	208/221 (94%)	202 (97%)	5 (2%)	1 (0%)	38	19
All	All	403/442 (91%)	391 (97%)	10 (2%)	2 (0%)	38	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	GLU
1	A	67	GLN

### 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	175/195 (90%)	159 (91%)	16 (9%)	14	3
1	B	185/195 (95%)	166 (90%)	19 (10%)	10	2
All	All	360/390 (92%)	325 (90%)	35 (10%)	12	3

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	29	GLU
1	A	33	LYS
1	A	36	LYS
1	A	39	GLU
1	A	42	ASP
1	A	43	LYS

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Mol	Chain	Res	Type
1	A	64	LYS
1	A	82	TYR
1	A	123	LEU
1	A	124	ILE
1	A	176	SER
1	A	177	SER
1	A	180	LEU
1	A	190	ASN
1	A	195	LYS
1	B	3	GLU
1	B	29	GLU
1	B	31	GLU
1	B	33	LYS
1	B	36	LYS
1	B	39	GLU
1	B	40	ASP
1	B	43	LYS
1	B	53	GLN
1	B	82	TYR
1	B	105	MET
1	B	111	VAL
1	B	120	LYS
1	B	123	LEU
1	B	126	GLU
1	B	143	HIS
1	B	170	LEU
1	B	176	SER
1	B	177	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	80	ASN
1	A	199	GLN
1	B	80	ASN
1	B	130	ASN
1	B	199	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

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, 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	198/221 (89%)	-0.12	6 (3%)	48	40	18, 35, 82, 136	1 (0%)
1	B	208/221 (94%)	-0.07	9 (4%)	34	27	17, 35, 85, 134	6 (2%)
All	All	406/442 (91%)	-0.09	15 (3%)	39	32	17, 35, 84, 136	7 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	8.9
1	A	110	PRO	5.1
1	A	209	ASP	4.7
1	A	208	MET	3.0
1	B	208	MET	2.9
1	B	39	GLU	2.7
1	B	46	ASN	2.6
1	B	3	GLU	2.6
1	B	209	ASP	2.4
1	A	109	LEU	2.4
1	B	176	SER	2.3
1	A	2	ALA	2.3
1	B	48	GLY	2.2
1	B	112	CYS	2.2
1	A	126	GLU	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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.