



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:40 PM GMT

PDB ID : 4FOL  
Title : S-formylglutathione hydrolase Variant H160I  
Authors : Legler, P.M.; Millard, C.B.  
Deposited on : 2012-06-20  
Resolution : 2.07 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

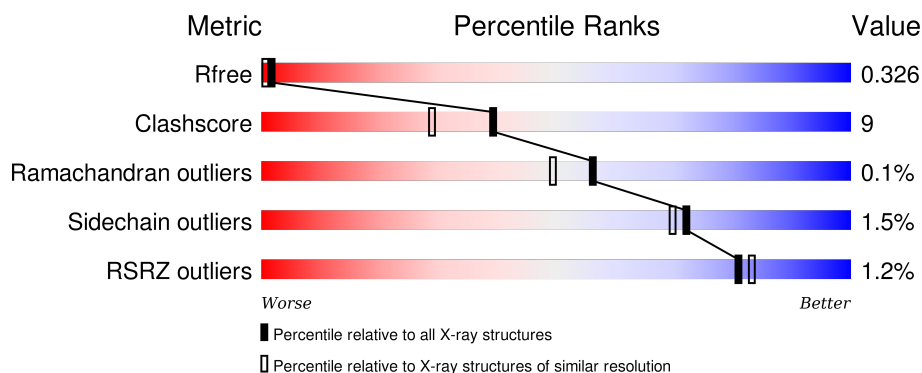
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	299	<div> <div></div> <div>75%18%• 5%</div> </div>
1	B	299	<div> <div></div> <div>77%17%• 5%</div> </div>
1	C	299	<div> <div>3%</div> <div>77%17%• 6%</div> </div>
1	D	299	<div> <div>%</div> <div>74%18%• 6%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9246 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 S-formylglutathione hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2270	1468	375	418	9			
1	B	283	Total	C	N	O	S	0	0	0
			2270	1468	374	419	9			
1	C	282	Total	C	N	O	S	0	0	0
			2261	1462	373	417	9			
1	D	282	Total	C	N	O	S	0	1	0
			2262	1464	370	419	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	ILE	HIS	ENGINEERED MUTATION	UNP P40363
B	160	ILE	HIS	ENGINEERED MUTATION	UNP P40363
C	160	ILE	HIS	ENGINEERED MUTATION	UNP P40363
D	160	ILE	HIS	ENGINEERED MUTATION	UNP P40363

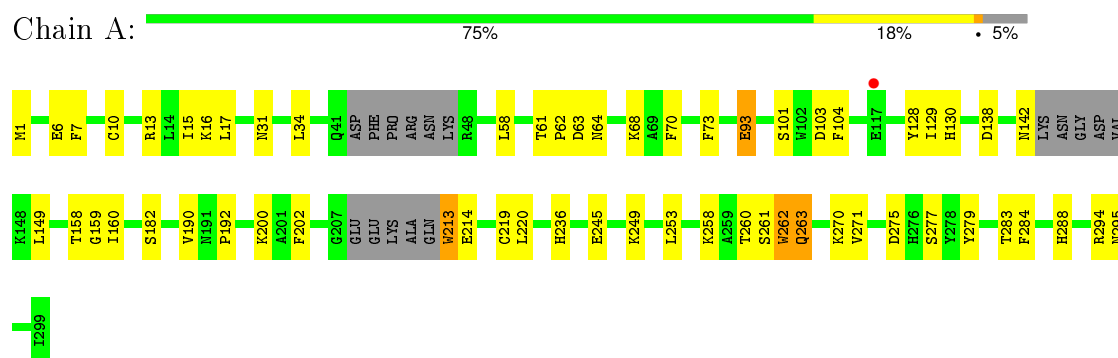
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	48	Total	O	0	0
			48	48		
2	B	45	Total	O	0	0
			45	45		
2	C	40	Total	O	0	0
			40	40		
2	D	50	Total	O	0	0
			50	50		

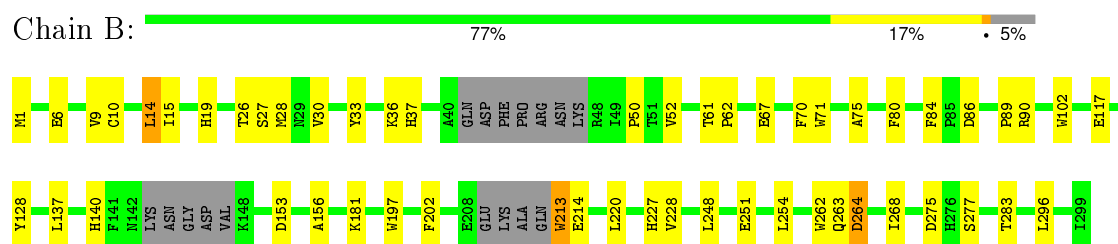
### 3 Residue-property plots

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.

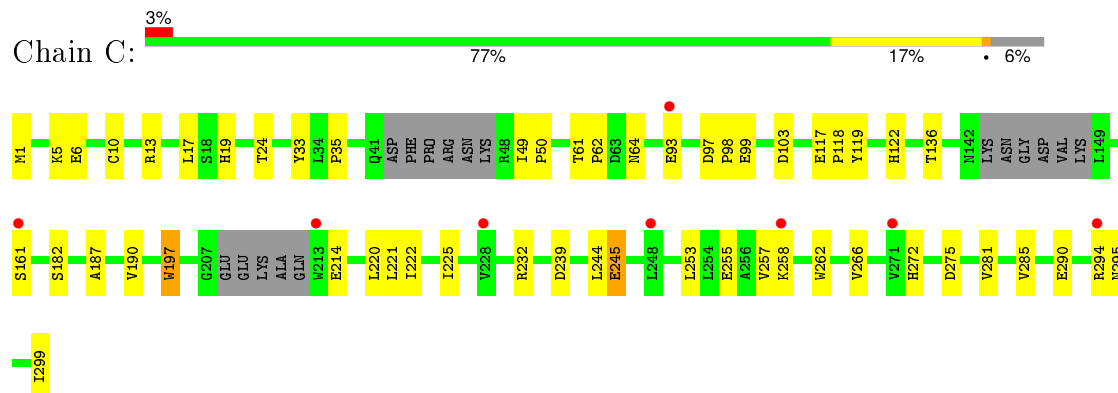
- Molecule 1: S-formylglutathione hydrolase



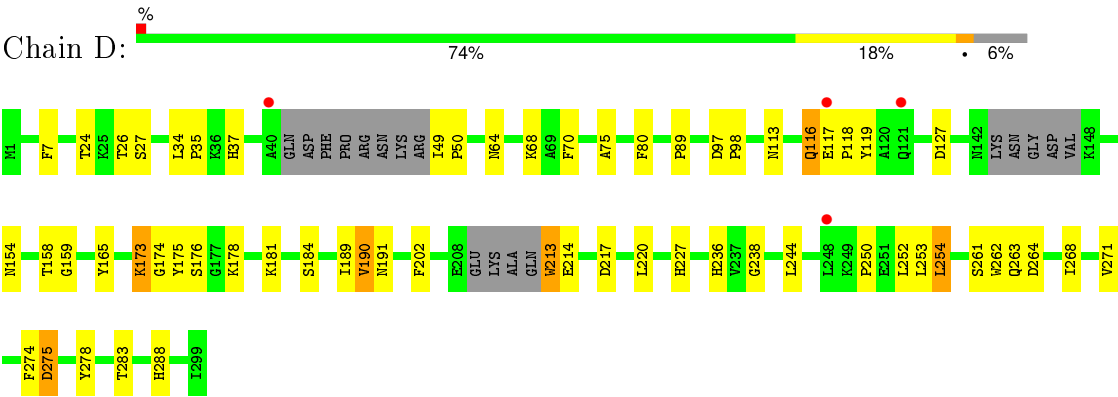
- Molecule 1: S-formylglutathione hydrolase



- Molecule 1: S-formylglutathione hydrolase



- Molecule 1: S-formylglutathione hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.30Å 119.74Å 169.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.73 – 2.07 61.73 – 2.07	Depositor EDS
% Data completeness (in resolution range)	90.9 (61.73-2.07) 90.9 (61.73-2.07)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.21	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.281 , 0.327 0.281 , 0.326	Depositor DCC
$R_{free}$ test set	4145 reflections (5.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.4	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 37.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 75321 reflections	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	9246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.28% 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	0.64	2/2339 (0.1%)	0.63	0/3169
1	B	0.66	5/2339 (0.2%)	0.64	1/3169 (0.0%)
1	C	0.64	2/2330 (0.1%)	0.61	0/3158
1	D	0.75	3/2334 (0.1%)	0.69	1/3163 (0.0%)
All	All	0.67	12/9342 (0.1%)	0.64	2/12659 (0.0%)

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	D	0	1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	262	TRP	NE1-CE2	-6.64	1.28	1.37
1	D	275	ASP	CB-CG	-6.06	1.39	1.51
1	B	197	TRP	CD2-CE2	5.41	1.47	1.41
1	B	262	TRP	CD2-CE2	5.34	1.47	1.41
1	B	102	TRP	CD2-CE2	5.19	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	LYS	N-CA-C	5.14	124.88	111.00
1	B	117	GLU	N-CA-C	5.08	124.71	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	116	GLN	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	2270	0	2167	54	0
1	B	2270	0	2165	34	0
1	C	2261	0	2154	33	0
1	D	2262	0	2157	46	0
2	A	48	0	0	3	0
2	B	45	0	0	3	0
2	C	40	0	0	0	0
2	D	50	0	0	2	0
All	All	9246	0	8643	157	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 9.

The worst 5 of 157 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:68:LYS:HE2	2:B:341:HOH:O	1.56	1.05
1:A:190:VAL:CG2	1:A:253:LEU:HB2	1.86	1.04
1:A:190:VAL:HG21	1:A:253:LEU:HB2	1.00	0.97
1:A:190:VAL:HG21	1:A:253:LEU:CB	1.96	0.92
1:D:271:VAL:HG12	1:D:274:PHE:HD2	1.37	0.90

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	275/299 (92%)	262 (95%)	13 (5%)	0	100	100
1	B	275/299 (92%)	260 (94%)	15 (6%)	0	100	100
1	C	274/299 (92%)	259 (94%)	14 (5%)	1 (0%)	39	28
1	D	275/299 (92%)	263 (96%)	12 (4%)	0	100	100
All	All	1099/1196 (92%)	1044 (95%)	54 (5%)	1 (0%)	56	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	245	GLU

### 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	241/255 (94%)	238 (99%)	3 (1%)	78	76
1	B	241/255 (94%)	237 (98%)	4 (2%)	68	65
1	C	240/255 (94%)	238 (99%)	2 (1%)	86	86
1	D	241/255 (94%)	236 (98%)	5 (2%)	61	57
All	All	963/1020 (94%)	949 (98%)	14 (2%)	72	70

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	264	ASP
1	C	190	VAL
1	D	190	VAL
1	B	251	GLU
1	D	176	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	64	ASN
1	C	194	ASN
1	D	194	ASN
1	C	130	HIS
1	C	191	ASN

### 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 [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	283/299 (94%)	0.30	1 (0%) 93 94	8, 13, 21, 31	0
1	B	283/299 (94%)	0.17	0 100 100	7, 12, 20, 25	0
1	C	282/299 (94%)	0.45	8 (2%) 56 62	9, 18, 31, 35	0
1	D	282/299 (94%)	0.21	4 (1%) 78 80	8, 13, 20, 28	0
All	All	1130/1196 (94%)	0.28	13 (1%) 81 83	7, 14, 25, 35	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	248	LEU	3.4
1	C	93	GLU	3.3
1	A	117	GLU	3.2
1	C	161	SER	2.7
1	C	228	VAL	2.4

### 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.