



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2018 – 09:59 am GMT

PDB ID : 1SOX  
Title : SULFITE OXIDASE FROM CHICKEN LIVER  
Authors : Kisker, C.; Schindelin, H.; Rees, D.C.  
Deposited on : 1997-12-31  
Resolution : 1.90 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](mailto: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  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

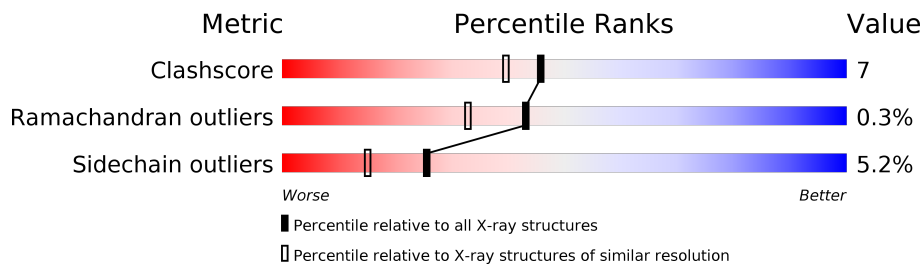
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	122078	6112 (1.90-1.90)
Ramachandran outliers	120005	6045 (1.90-1.90)
Sidechain outliers	119972	6045 (1.90-1.90)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	466	
1	B	466	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8189 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 SULFITE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	6	0
			3613	2293	654	659	7			
1	B	458	Total	C	N	O	S	0	6	0
			3577	2271	641	658	7			

There are 16 discrepancies between the modelled and reference sequences:

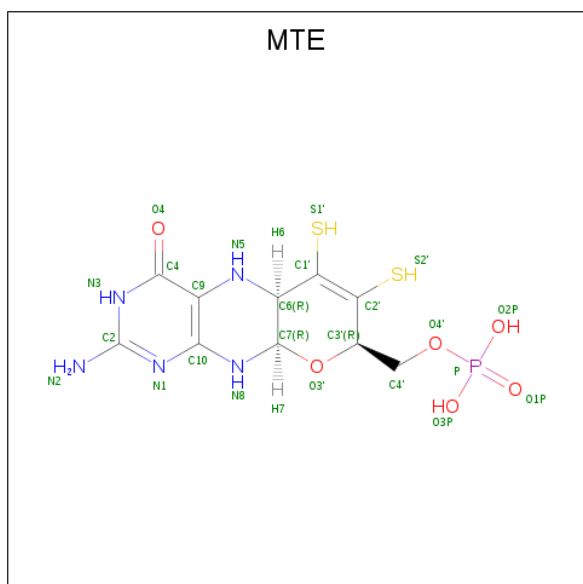
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLU	ARG	CORRECTION	UNP P07850
A	?	-	ARG	DELETION	UNP P07850
A	161	GLY	ARG	CORRECTION	UNP P07850
A	218	ARG	SER	CORRECTION	UNP P07850
A	235	GLU	GLY	CORRECTION	UNP P07850
A	236	TRP	GLU	CORRECTION	UNP P07850
A	284	GLY	ARG	CORRECTION	UNP P07850
A	316	HIS	ARG	CORRECTION	UNP P07850
B	6	GLU	ARG	CORRECTION	UNP P07850
B	?	-	ARG	DELETION	UNP P07850
B	161	GLY	ARG	CORRECTION	UNP P07850
B	218	ARG	SER	CORRECTION	UNP P07850
B	235	GLU	GLY	CORRECTION	UNP P07850
B	236	TRP	GLU	CORRECTION	UNP P07850
B	284	GLY	ARG	CORRECTION	UNP P07850
B	316	HIS	ARG	CORRECTION	UNP P07850

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula:  $C_{10}H_{14}N_5O_6PS_2$ ).

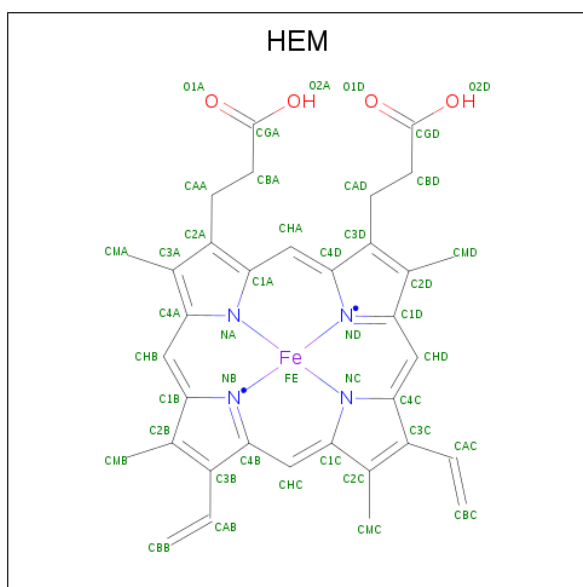


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
3	B	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

- Molecule 4 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mo 1 1	0	0
4	A	1	Total Mo 1 1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



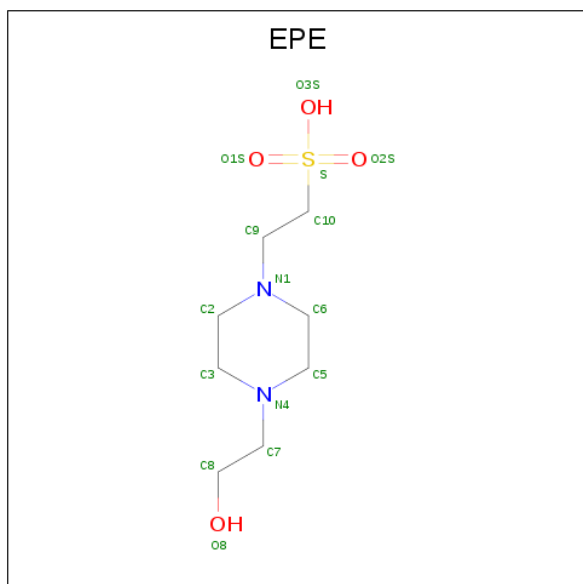
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	417	Total 417	O 417	0	0
8	B	405	Total 405	O 405	0	0

### 3 Residue-property plots

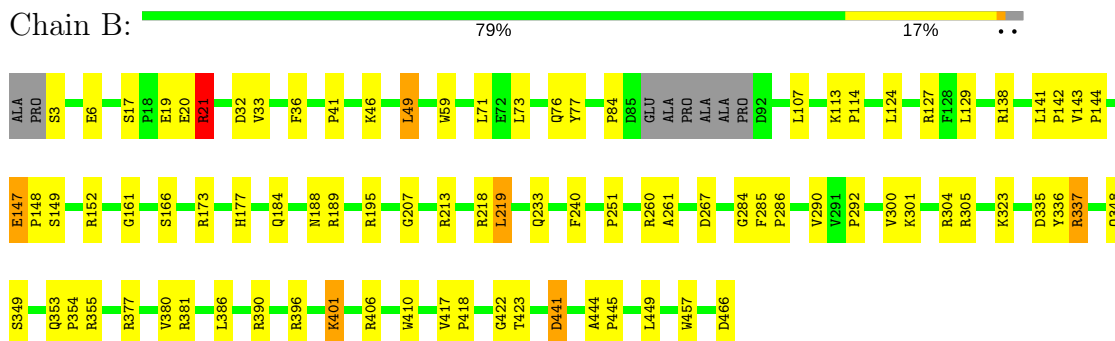
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

#### • Molecule 1: SULFITE OXIDASE



#### • Molecule 1: SULFITE OXIDASE





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.12Å 197.69Å 56.01Å 90.00° 94.23° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	89.2 (50.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.175 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8189	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MO, SO4, HEM, EPE, MTE

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	0.49	0/3749	1.10	18/5128 (0.4%)
1	B	0.48	0/3712	1.08	20/5078 (0.4%)
All	All	0.48	0/7461	1.09	38/10206 (0.4%)

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	A	355	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	A	355	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	355	ARG	CD-NE-CZ	8.26	135.17	123.60
1	A	337	ARG	NE-CZ-NH1	8.14	124.37	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	3613	0	3503	50	0
1	B	3577	0	3456	49	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	24	0	10	0	0
3	B	24	0	10	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	43	0	30	2	0
5	B	43	0	30	3	0
6	A	6	0	8	0	0
7	B	15	0	18	2	0
8	A	417	0	0	0	0
8	B	405	0	0	0	0
All	All	8189	0	7065	98	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 7.

The worst 5 of 98 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:161:GLY:HA3	7:B:911:EPE:H52	1.57	0.83
1:B:386:LEU:HD11	1:B:417:VAL:HG21	1.67	0.76
1:A:124:LEU:HD11	1:A:207:GLY:HA2	1.69	0.73
1:A:305[B]:ARG:HH11	1:A:305[B]:ARG:HG3	1.51	0.73
1:B:335:ASP:OD1	1:B:337:ARG:HD3	1.89	0.71

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	465/466 (100%)	453 (97%)	11 (2%)	1 (0%)	49	40
1	B	460/466 (99%)	448 (97%)	10 (2%)	2 (0%)	36	25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	925/932 (99%)	901 (97%)	21 (2%)	3 (0%)	43	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	B	21	ARG
1	B	84	PRO

### 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	379/377 (100%)	361 (95%)	18 (5%)	29	18
1	B	377/377 (100%)	355 (94%)	22 (6%)	22	12
All	All	756/754 (100%)	716 (95%)	40 (5%)	25	14

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	SER
1	B	59	TRP
1	B	410	TRP
1	B	21	ARG
1	B	71	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	A	465	GLN
1	B	343	GLN
1	A	343	GLN
1	B	319	GLN

### 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 ⓘ

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	MTE	A	501	4	21,26,26	5.76	10 (47%)	19,40,40	3.02	9 (47%)
5	HEM	A	502	1	27,50,50	2.05	5 (18%)	17,82,82	3.12	7 (41%)
2	SO4	A	503	-	4,4,4	1.05	0	6,6,6	0.28	0
2	SO4	A	504	-	4,4,4	1.11	0	6,6,6	0.24	0
6	GOL	A	912	-	5,5,5	0.10	0	5,5,5	0.28	0
3	MTE	B	501	4	21,26,26	5.71	12 (57%)	19,40,40	3.04	7 (36%)
5	HEM	B	502	1	27,50,50	1.87	4 (14%)	17,82,82	2.19	6 (35%)
2	SO4	B	503	-	4,4,4	1.01	0	6,6,6	0.40	0
2	SO4	B	504	-	4,4,4	1.09	0	6,6,6	0.32	0
7	EPE	B	911	-	15,15,15	1.86	2 (13%)	18,20,20	2.19	7 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MTE	A	501	4	-	0/6/34/34	0/3/3/3
5	HEM	A	502	1	-	0/6/54/54	0/0/8/8
2	SO4	A	503	-	-	0/0/0/0	0/0/0/0
2	SO4	A	504	-	-	0/0/0/0	0/0/0/0
6	GOL	A	912	-	-	0/4/4/4	0/0/0/0
3	MTE	B	501	4	-	0/6/34/34	0/3/3/3
5	HEM	B	502	1	-	0/6/54/54	0/0/8/8
2	SO4	B	503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	504	-	-	0/0/0/0	0/0/0/0
7	EPE	B	911	-	-	0/9/19/19	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	MTE	C4'-C3'	-7.90	1.40	1.52
3	B	501	MTE	C4'-C3'	-7.25	1.41	1.52
3	A	501	MTE	P-O4'	-6.85	1.38	1.60
3	B	501	MTE	P-O4'	-6.28	1.40	1.60
5	A	502	HEM	C3B-C2B	-5.16	1.33	1.40

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	MTE	O3'-C7-C6	-6.28	104.77	108.96
3	B	501	MTE	O3'-C7-C6	-4.74	105.80	108.96
7	B	911	EPE	O3S-S-O1S	-4.59	100.06	111.27
3	B	501	MTE	N3-C2-N1	-4.45	118.36	125.43
5	A	502	HEM	CMD-C2D-C1D	-3.99	122.32	128.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	HEM	2	0
5	B	502	HEM	3	0
7	B	911	EPE	2	0

## 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.