



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 22, 2018 – 10:36 AM EST

PDB ID : 5D96  
Title : Oxidoreductase Fragment of Mouse QSOX1 in Complex with a FAb Fragment from an Antibody Targeting Mouse and Human QSOX1  
Authors : Fass, D.; Grossman, I.  
Deposited on : 2015-08-18  
Resolution : 2.30 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030736

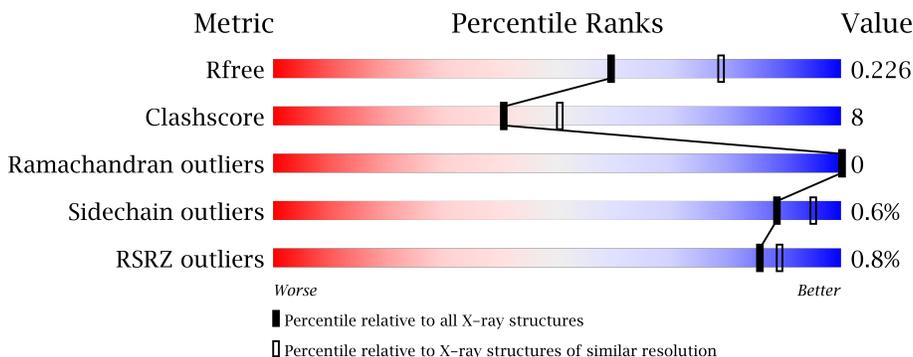
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	244	 2% 79% 18%
1	D	244	 1% 77% 18%
2	B	214	 82% 18%
2	I	214	 84% 15%
3	C	220	 1% 77% 19%

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Mol	Chain	Length	Quality of chain
3	J	220	 80% 17%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10605 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 Sulphydryl oxidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	234	Total	C	N	O	S	0	0	0
			1807	1152	307	341	7			
1	A	237	Total	C	N	O	S	0	1	0
			1846	1177	314	348	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	32	GLY	-	expression tag	UNP Q8BND5
D	33	SER	-	expression tag	UNP Q8BND5
D	34	HIS	-	expression tag	UNP Q8BND5
D	35	MET	-	expression tag	UNP Q8BND5
A	32	GLY	-	expression tag	UNP Q8BND5
A	33	SER	-	expression tag	UNP Q8BND5
A	34	HIS	-	expression tag	UNP Q8BND5
A	35	MET	-	expression tag	UNP Q8BND5

- Molecule 2 is a protein called Light chain of Fab fragment from an antibody targeting mouse and human QSOX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	214	Total	C	N	O	S	0	1	0
			1656	1030	280	337	9			
2	B	214	Total	C	N	O	S	0	0	0
			1651	1027	279	336	9			

- Molecule 3 is a protein called Heavy chain of Fab fragment from an antibody targeting mouse and human QSOX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	J	215	Total	C	N	O	S	0	0	0
			1612	1021	267	315	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	214	1608	1019	266	314	9	0	0	0

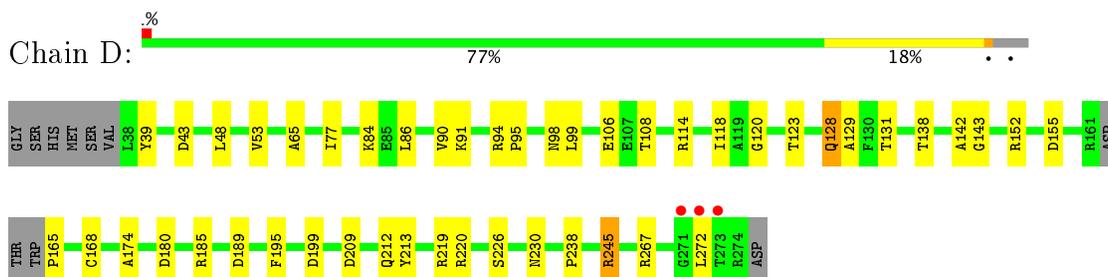
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	75	Total 75	O 75	0	0
4	I	77	Total 77	O 77	0	0
4	J	71	Total 71	O 71	0	0
4	A	81	Total 81	O 81	0	0
4	B	66	Total 66	O 66	0	0
4	C	55	Total 55	O 55	0	0

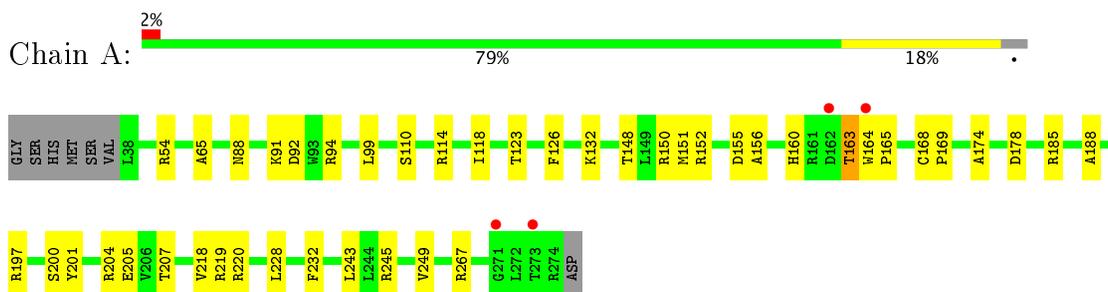
### 3 Residue-property plots [i](#)

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.

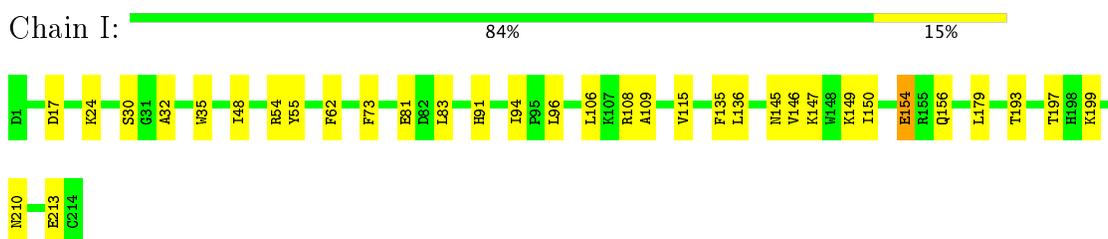
- Molecule 1: Sulfhydryl oxidase 1



- Molecule 1: Sulfhydryl oxidase 1



- Molecule 2: Light chain of Fab fragment from an antibody targeting mouse and human QSOX1



- Molecule 2: Light chain of Fab fragment from an antibody targeting mouse and human QSOX1

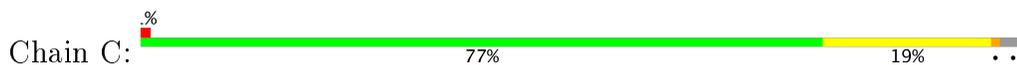




- Molecule 3: Heavy chain of Fab fragment from an antibody targeting mouse and human QSOX1



- Molecule 3: Heavy chain of Fab fragment from an antibody targeting mouse and human QSOX1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.80Å 204.77Å 44.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.42 – 2.30 27.42 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.42-2.30) 96.8 (27.42-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.31Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.167 , 0.228 0.168 , 0.226	Depositor DCC
$R_{free}$ test set	1927 reflections (3.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtrriage
Anisotropy	0.179	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 24.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.419 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.27	0/1896	0.49	0/2589
1	D	0.28	0/1850	0.52	0/2522
2	B	0.26	0/1686	0.50	0/2287
2	I	0.28	0/1694	0.52	0/2298
3	C	0.27	0/1648	0.54	1/2250 (0.0%)
3	J	0.25	0/1652	0.53	0/2255
All	All	0.27	0/10426	0.52	1/14201 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	67	LEU	CA-CB-CG	5.59	128.17	115.30

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	1846	0	1790	31	1
1	D	1807	0	1758	42	0
2	B	1651	0	1585	28	0
2	I	1656	0	1591	23	1
3	C	1608	0	1592	24	0
3	J	1612	0	1595	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	81	0	0	4	0
4	B	66	0	0	1	0
4	C	55	0	0	2	1
4	D	75	0	0	4	0
4	I	77	0	0	1	0
4	J	71	0	0	1	1
All	All	10605	0	9911	164	2

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 8.

The worst 5 of 164 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:D:226:SER:OG	2:B:108:ARG:NH1	2.05	0.89
2:B:149:LYS:HB2	2:B:193:THR:HB	1.55	0.88
1:A:204:ARG:HG3	1:A:220:ARG:HD2	1.53	0.88
1:D:230:ASN:ND2	2:B:169:LYS:O	2.14	0.81
1:D:128:GLN:HA	1:D:128:GLN:HE21	1.48	0.77

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:301:HOH:O	4:C:333:HOH:O[2_554]	2.09	0.11
2:I:17:ASP:OD1	1:A:197:ARG:NH1[1_556]	2.13	0.07

## 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	236/244 (97%)	232 (98%)	4 (2%)	0	100	100
1	D	230/244 (94%)	226 (98%)	4 (2%)	0	100	100
2	B	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
2	I	213/214 (100%)	207 (97%)	6 (3%)	0	100	100
3	C	210/220 (96%)	206 (98%)	4 (2%)	0	100	100
3	J	211/220 (96%)	209 (99%)	2 (1%)	0	100	100
All	All	1312/1356 (97%)	1287 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	200/207 (97%)	199 (100%)	1 (0%)	91	96
1	D	195/207 (94%)	193 (99%)	2 (1%)	80	90
2	B	188/188 (100%)	188 (100%)	0	100	100
2	I	189/188 (100%)	188 (100%)	1 (0%)	91	96
3	C	187/191 (98%)	185 (99%)	2 (1%)	78	89
3	J	187/191 (98%)	186 (100%)	1 (0%)	91	96
All	All	1146/1172 (98%)	1139 (99%)	7 (1%)	89	95

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	200	CYS
3	C	138	ASN
1	A	163	THR
1	D	245	ARG
3	C	43	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	98	ASN
1	D	128	GLN
2	I	8	HIS
1	A	75	HIS

### 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	237/244 (97%)	-0.17	4 (1%) 70 76	20, 35, 51, 70	0
1	D	234/244 (95%)	-0.22	3 (1%) 77 81	25, 34, 51, 69	1 (0%)
2	B	214/214 (100%)	-0.30	0 100 100	22, 34, 49, 57	0
2	I	214/214 (100%)	-0.38	0 100 100	23, 32, 43, 53	0
3	C	214/220 (97%)	-0.27	2 (0%) 84 87	23, 35, 52, 65	0
3	J	215/220 (97%)	-0.31	1 (0%) 90 93	22, 33, 45, 54	0
All	All	1328/1356 (97%)	-0.27	10 (0%) 86 89	20, 34, 49, 70	1 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	GLY	4.9
3	C	219	ASP	3.6
1	A	273	THR	3.3
3	J	42	GLY	3.1
1	A	162	ASP	2.8

### 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

There are no such residues in this entry.