



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:46 AM UTC

PDB ID : 3SBC / pdb_00003sbc
Title : Crystal structure of Saccharomyces cerevisiae TSA1C47S mutant protein
Authors : Tairum Jr., C.A.; Horta, B.B.; Netto, L.E.S.; Oliveira, M.A.
Deposited on : 2011-06-03
Resolution : 2.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

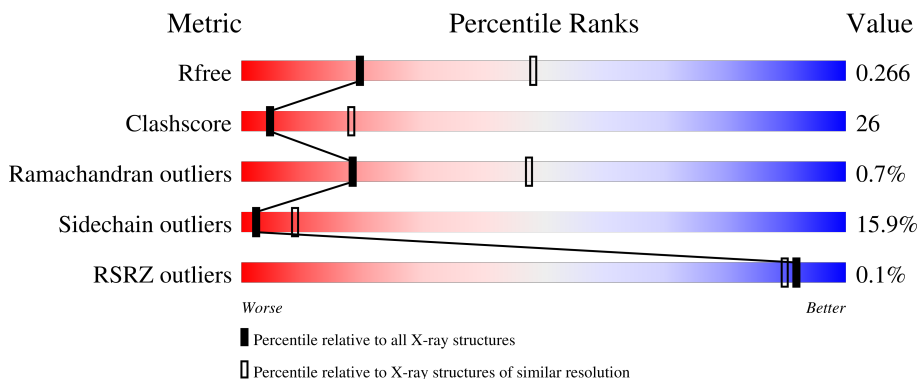
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.






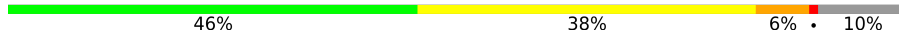
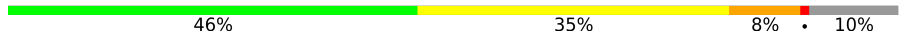
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	216	 55% 29% 7% 10%
1	B	216	 48% 36% 7% 9%
1	C	216	 41% 43% 7% 9%
1	D	216	 42% 40% 6% • 10%
1	E	216	 47% 32% 10% • 10%

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Mol	Chain	Length	Quality of chain
1	F	216	 40% 42% 6% • 10%
1	G	216	 48% 36% 6% • 10%
1	H	216	 48% 31% 10% • 10%
1	I	216	 46% 38% 6% • 10%
1	J	216	 46% 35% 8% • 10%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15429 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 Peroxiredoxin TSA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	195	1520	980	250	289	1	0	1	0
1	B	197	1524	984	250	289	1	0	1	0
1	C	196	1498	967	245	285	1	0	0	0
1	D	194	1496	968	246	281	1	0	0	0
1	E	195	1493	963	243	286	1	0	0	0
1	F	194	1480	955	241	283	1	0	0	0
1	G	195	1501	969	245	286	1	0	0	0
1	H	195	1514	977	247	289	1	0	1	0
1	I	195	1497	966	244	286	1	0	0	0
1	J	195	1506	972	246	287	1	0	1	0

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P34760
A	-19	GLY	-	expression tag	UNP P34760
A	-18	SER	-	expression tag	UNP P34760
A	-17	SER	-	expression tag	UNP P34760
A	-16	HIS	-	expression tag	UNP P34760
A	-15	HIS	-	expression tag	UNP P34760
A	-14	HIS	-	expression tag	UNP P34760
A	-13	HIS	-	expression tag	UNP P34760
A	-12	HIS	-	expression tag	UNP P34760

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	HIS	-	expression tag	UNP P34760
A	-10	SER	-	expression tag	UNP P34760
A	-9	SER	-	expression tag	UNP P34760
A	-8	GLY	-	expression tag	UNP P34760
A	-7	LEU	-	expression tag	UNP P34760
A	-6	VAL	-	expression tag	UNP P34760
A	-5	PRO	-	expression tag	UNP P34760
A	-4	ARG	-	expression tag	UNP P34760
A	-3	GLY	-	expression tag	UNP P34760
A	-2	SER	-	expression tag	UNP P34760
A	-1	HIS	-	expression tag	UNP P34760
A	47	SER	CYS	engineered mutation	UNP P34760
B	-20	MET	-	expression tag	UNP P34760
B	-19	GLY	-	expression tag	UNP P34760
B	-18	SER	-	expression tag	UNP P34760
B	-17	SER	-	expression tag	UNP P34760
B	-16	HIS	-	expression tag	UNP P34760
B	-15	HIS	-	expression tag	UNP P34760
B	-14	HIS	-	expression tag	UNP P34760
B	-13	HIS	-	expression tag	UNP P34760
B	-12	HIS	-	expression tag	UNP P34760
B	-11	HIS	-	expression tag	UNP P34760
B	-10	SER	-	expression tag	UNP P34760
B	-9	SER	-	expression tag	UNP P34760
B	-8	GLY	-	expression tag	UNP P34760
B	-7	LEU	-	expression tag	UNP P34760
B	-6	VAL	-	expression tag	UNP P34760
B	-5	PRO	-	expression tag	UNP P34760
B	-4	ARG	-	expression tag	UNP P34760
B	-3	GLY	-	expression tag	UNP P34760
B	-2	SER	-	expression tag	UNP P34760
B	-1	HIS	-	expression tag	UNP P34760
B	47	SER	CYS	engineered mutation	UNP P34760
C	-20	MET	-	expression tag	UNP P34760
C	-19	GLY	-	expression tag	UNP P34760
C	-18	SER	-	expression tag	UNP P34760
C	-17	SER	-	expression tag	UNP P34760
C	-16	HIS	-	expression tag	UNP P34760
C	-15	HIS	-	expression tag	UNP P34760
C	-14	HIS	-	expression tag	UNP P34760
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	HIS	-	expression tag	UNP P34760
C	-10	SER	-	expression tag	UNP P34760
C	-9	SER	-	expression tag	UNP P34760
C	-8	GLY	-	expression tag	UNP P34760
C	-7	LEU	-	expression tag	UNP P34760
C	-6	VAL	-	expression tag	UNP P34760
C	-5	PRO	-	expression tag	UNP P34760
C	-4	ARG	-	expression tag	UNP P34760
C	-3	GLY	-	expression tag	UNP P34760
C	-2	SER	-	expression tag	UNP P34760
C	-1	HIS	-	expression tag	UNP P34760
C	47	SER	CYS	engineered mutation	UNP P34760
D	-20	MET	-	expression tag	UNP P34760
D	-19	GLY	-	expression tag	UNP P34760
D	-18	SER	-	expression tag	UNP P34760
D	-17	SER	-	expression tag	UNP P34760
D	-16	HIS	-	expression tag	UNP P34760
D	-15	HIS	-	expression tag	UNP P34760
D	-14	HIS	-	expression tag	UNP P34760
D	-13	HIS	-	expression tag	UNP P34760
D	-12	HIS	-	expression tag	UNP P34760
D	-11	HIS	-	expression tag	UNP P34760
D	-10	SER	-	expression tag	UNP P34760
D	-9	SER	-	expression tag	UNP P34760
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D	-5	PRO	-	expression tag	UNP P34760
D	-4	ARG	-	expression tag	UNP P34760
D	-3	GLY	-	expression tag	UNP P34760
D	-2	SER	-	expression tag	UNP P34760
D	-1	HIS	-	expression tag	UNP P34760
D	47	SER	CYS	engineered mutation	UNP P34760
E	-20	MET	-	expression tag	UNP P34760
E	-19	GLY	-	expression tag	UNP P34760
E	-18	SER	-	expression tag	UNP P34760
E	-17	SER	-	expression tag	UNP P34760
E	-16	HIS	-	expression tag	UNP P34760
E	-15	HIS	-	expression tag	UNP P34760
E	-14	HIS	-	expression tag	UNP P34760
E	-13	HIS	-	expression tag	UNP P34760
E	-12	HIS	-	expression tag	UNP P34760

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	HIS	-	expression tag	UNP P34760
E	-10	SER	-	expression tag	UNP P34760
E	-9	SER	-	expression tag	UNP P34760
E	-8	GLY	-	expression tag	UNP P34760
E	-7	LEU	-	expression tag	UNP P34760
E	-6	VAL	-	expression tag	UNP P34760
E	-5	PRO	-	expression tag	UNP P34760
E	-4	ARG	-	expression tag	UNP P34760
E	-3	GLY	-	expression tag	UNP P34760
E	-2	SER	-	expression tag	UNP P34760
E	-1	HIS	-	expression tag	UNP P34760
E	47	SER	CYS	engineered mutation	UNP P34760
F	-20	MET	-	expression tag	UNP P34760
F	-19	GLY	-	expression tag	UNP P34760
F	-18	SER	-	expression tag	UNP P34760
F	-17	SER	-	expression tag	UNP P34760
F	-16	HIS	-	expression tag	UNP P34760
F	-15	HIS	-	expression tag	UNP P34760
F	-14	HIS	-	expression tag	UNP P34760
F	-13	HIS	-	expression tag	UNP P34760
F	-12	HIS	-	expression tag	UNP P34760
F	-11	HIS	-	expression tag	UNP P34760
F	-10	SER	-	expression tag	UNP P34760
F	-9	SER	-	expression tag	UNP P34760
F	-8	GLY	-	expression tag	UNP P34760
F	-7	LEU	-	expression tag	UNP P34760
F	-6	VAL	-	expression tag	UNP P34760
F	-5	PRO	-	expression tag	UNP P34760
F	-4	ARG	-	expression tag	UNP P34760
F	-3	GLY	-	expression tag	UNP P34760
F	-2	SER	-	expression tag	UNP P34760
F	-1	HIS	-	expression tag	UNP P34760
F	47	SER	CYS	engineered mutation	UNP P34760
G	-20	MET	-	expression tag	UNP P34760
G	-19	GLY	-	expression tag	UNP P34760
G	-18	SER	-	expression tag	UNP P34760
G	-17	SER	-	expression tag	UNP P34760
G	-16	HIS	-	expression tag	UNP P34760
G	-15	HIS	-	expression tag	UNP P34760
G	-14	HIS	-	expression tag	UNP P34760
G	-13	HIS	-	expression tag	UNP P34760
G	-12	HIS	-	expression tag	UNP P34760

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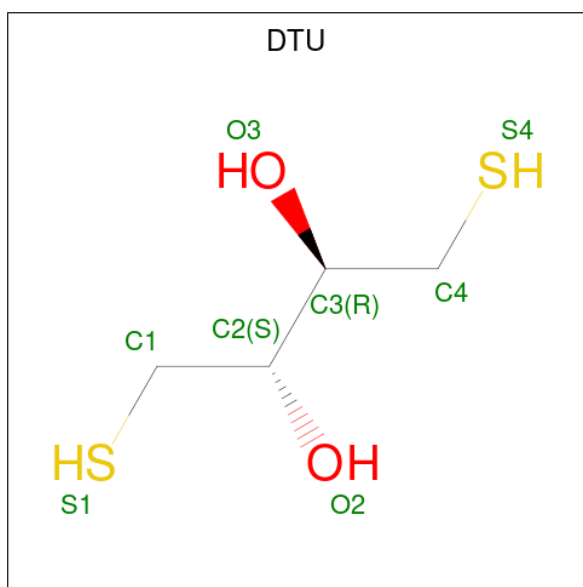
Chain	Residue	Modelled	Actual	Comment	Reference
G	-11	HIS	-	expression tag	UNP P34760
G	-10	SER	-	expression tag	UNP P34760
G	-9	SER	-	expression tag	UNP P34760
G	-8	GLY	-	expression tag	UNP P34760
G	-7	LEU	-	expression tag	UNP P34760
G	-6	VAL	-	expression tag	UNP P34760
G	-5	PRO	-	expression tag	UNP P34760
G	-4	ARG	-	expression tag	UNP P34760
G	-3	GLY	-	expression tag	UNP P34760
G	-2	SER	-	expression tag	UNP P34760
G	-1	HIS	-	expression tag	UNP P34760
G	47	SER	CYS	engineered mutation	UNP P34760
H	-20	MET	-	expression tag	UNP P34760
H	-19	GLY	-	expression tag	UNP P34760
H	-18	SER	-	expression tag	UNP P34760
H	-17	SER	-	expression tag	UNP P34760
H	-16	HIS	-	expression tag	UNP P34760
H	-15	HIS	-	expression tag	UNP P34760
H	-14	HIS	-	expression tag	UNP P34760
H	-13	HIS	-	expression tag	UNP P34760
H	-12	HIS	-	expression tag	UNP P34760
H	-11	HIS	-	expression tag	UNP P34760
H	-10	SER	-	expression tag	UNP P34760
H	-9	SER	-	expression tag	UNP P34760
H	-8	GLY	-	expression tag	UNP P34760
H	-7	LEU	-	expression tag	UNP P34760
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H	-4	ARG	-	expression tag	UNP P34760
H	-3	GLY	-	expression tag	UNP P34760
H	-2	SER	-	expression tag	UNP P34760
H	-1	HIS	-	expression tag	UNP P34760
H	47	SER	CYS	engineered mutation	UNP P34760
I	-20	MET	-	expression tag	UNP P34760
I	-19	GLY	-	expression tag	UNP P34760
I	-18	SER	-	expression tag	UNP P34760
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I	-16	HIS	-	expression tag	UNP P34760
I	-15	HIS	-	expression tag	UNP P34760
I	-14	HIS	-	expression tag	UNP P34760
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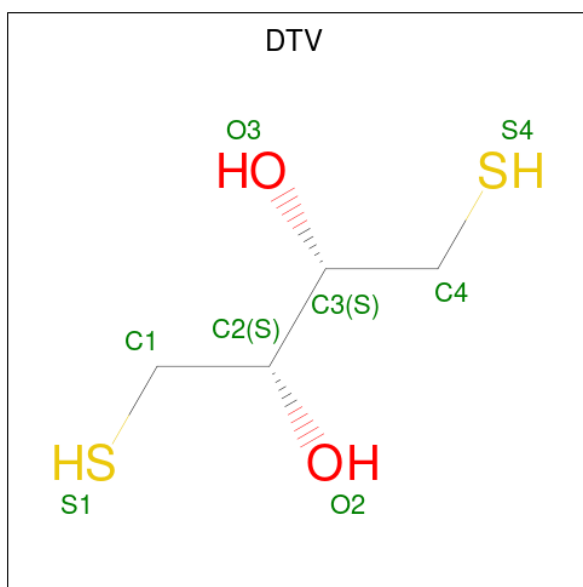
Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	expression tag	UNP P34760
I	-10	SER	-	expression tag	UNP P34760
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I	-8	GLY	-	expression tag	UNP P34760
I	-7	LEU	-	expression tag	UNP P34760
I	-6	VAL	-	expression tag	UNP P34760
I	-5	PRO	-	expression tag	UNP P34760
I	-4	ARG	-	expression tag	UNP P34760
I	-3	GLY	-	expression tag	UNP P34760
I	-2	SER	-	expression tag	UNP P34760
I	-1	HIS	-	expression tag	UNP P34760
I	47	SER	CYS	engineered mutation	UNP P34760
J	-20	MET	-	expression tag	UNP P34760
J	-19	GLY	-	expression tag	UNP P34760
J	-18	SER	-	expression tag	UNP P34760
J	-17	SER	-	expression tag	UNP P34760
J	-16	HIS	-	expression tag	UNP P34760
J	-15	HIS	-	expression tag	UNP P34760
J	-14	HIS	-	expression tag	UNP P34760
J	-13	HIS	-	expression tag	UNP P34760
J	-12	HIS	-	expression tag	UNP P34760
J	-11	HIS	-	expression tag	UNP P34760
J	-10	SER	-	expression tag	UNP P34760
J	-9	SER	-	expression tag	UNP P34760
J	-8	GLY	-	expression tag	UNP P34760
J	-7	LEU	-	expression tag	UNP P34760
J	-6	VAL	-	expression tag	UNP P34760
J	-5	PRO	-	expression tag	UNP P34760
J	-4	ARG	-	expression tag	UNP P34760
J	-3	GLY	-	expression tag	UNP P34760
J	-2	SER	-	expression tag	UNP P34760
J	-1	HIS	-	expression tag	UNP P34760
J	47	SER	CYS	engineered mutation	UNP P34760

- Molecule 2 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (CCD ID: DTU) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	S	0	0
			8	4	2	2		
2	E	1	Total	C	O	S	0	0
			8	4	2	2		
2	G	1	Total	C	O	S	0	0
			8	4	2	2		
2	H	1	Total	C	O	S	0	0
			8	4	2	2		
2	J	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 3 is (2S,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (CCD ID: DTV) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 4 is water.

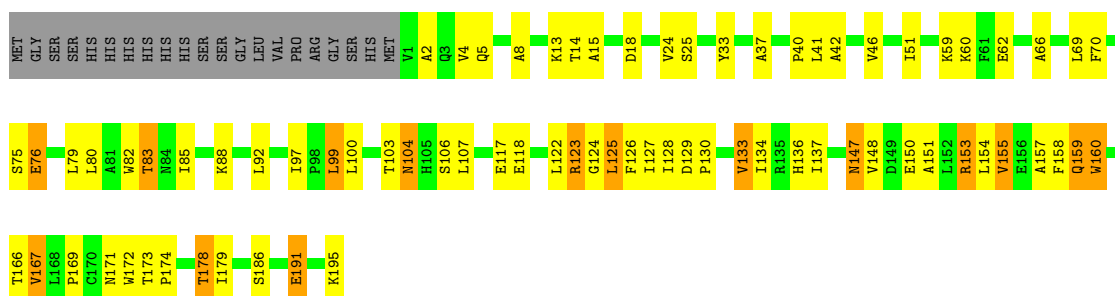
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	52	Total	O	0	0
			52	52		
4	C	27	Total	O	0	0
			27	27		
4	D	32	Total	O	0	0
			32	32		
4	E	20	Total	O	0	0
			20	20		
4	F	33	Total	O	0	0
			33	33		
4	G	48	Total	O	0	0
			48	48		
4	H	39	Total	O	0	0
			39	39		
4	I	30	Total	O	0	0
			30	30		
4	J	23	Total	O	0	0
			23	23		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

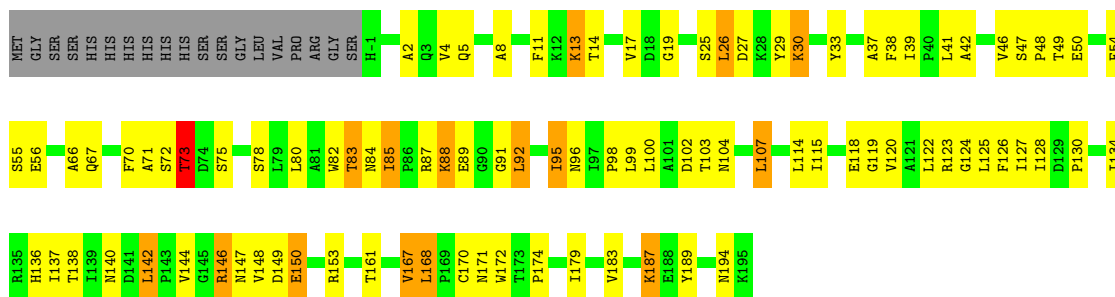
- Molecule 1: Peroxiredoxin TSA1

Chain A: 



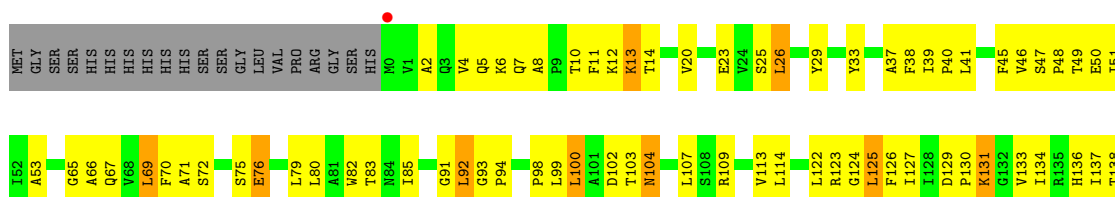
- Molecule 1: Peroxiredoxin TSA1

Chain B: 



- Molecule 1: Peroxiredoxin TSA1

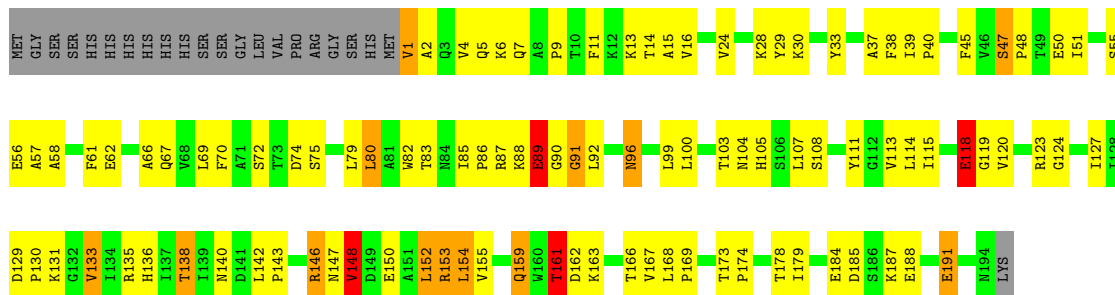
Chain C: 





- Molecule 1: Peroxiredoxin TSA1

Chain D: 42% 40% 6% 10%



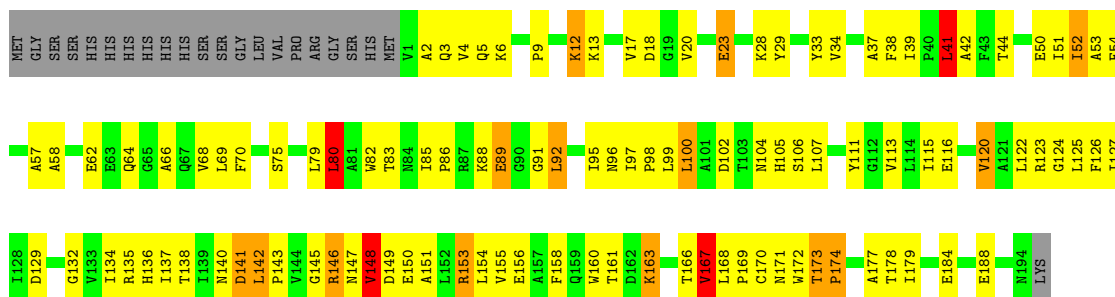
- Molecule 1: Peroxiredoxin TSA1

Chain E: 47% 32% 10% 10%



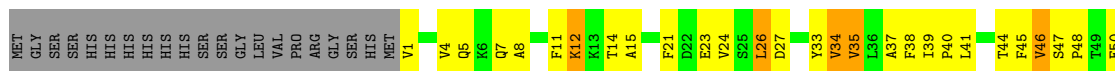
- Molecule 1: Peroxiredoxin TSA1

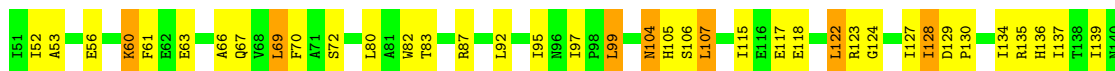
Chain F: 40% 42% 6% 10%



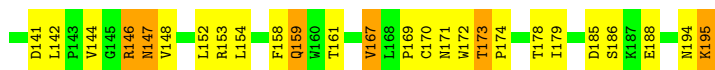
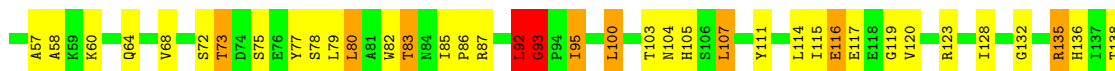
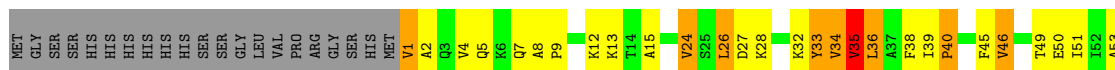
- Molecule 1: Peroxiredoxin TSA1

Chain G: 48% 36% 6% 10%

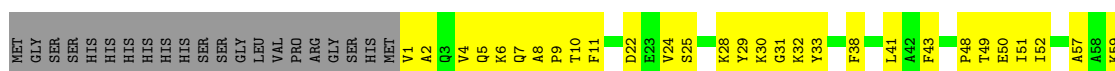




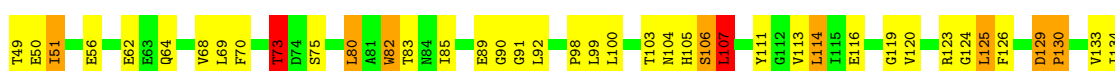
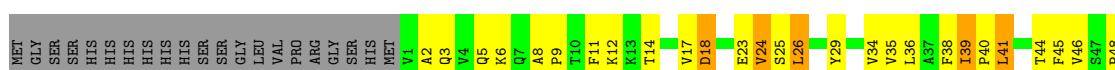
• Molecule 1: Peroxiredoxin TSA1



• Molecule 1: Peroxiredoxin TSA1



• Molecule 1: Peroxiredoxin TSA1



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	239.98Å 51.96Å 192.35Å 90.00° 92.33° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.80) 97.6 (50.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.202 , 0.274 0.197 , 0.266	Depositor DCC
R_{free} test set	2933 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtrriage
Anisotropy	0.223	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 22.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtrriage
Reported twinning fraction	0.937 for H, K, L 0.063 for -h,-k,l	Depositor
Outliers	0 of 58039 reflections	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15429	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DTU, DTU

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	0.96	0/1554	1.09	5/2117 (0.2%)
1	B	0.98	0/1558	1.18	4/2123 (0.2%)
1	C	0.88	0/1532	1.12	1/2092 (0.0%)
1	D	0.98	0/1530	1.24	8/2085 (0.4%)
1	E	0.82	0/1527	1.16	9/2086 (0.4%)
1	F	0.94	0/1514	1.21	5/2070 (0.2%)
1	G	0.91	0/1535	1.14	5/2094 (0.2%)
1	H	0.99	1/1548 (0.1%)	1.23	7/2110 (0.3%)
1	I	0.87	0/1531	1.11	7/2090 (0.3%)
1	J	0.96	0/1540	1.20	8/2101 (0.4%)
All	All	0.93	1/15369 (0.0%)	1.17	59/20968 (0.3%)

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	2
1	H	0	1
1	I	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	35	VAL	CA-CB	5.13	1.60	1.54

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	GLN	N-CA-C	-7.64	102.95	111.28
1	E	179	ILE	N-CA-C	7.48	119.09	108.17
1	H	93	GLY	CA-C-N	-7.02	111.06	119.84
1	H	93	GLY	C-N-CA	-7.02	111.06	119.84
1	A	155	VAL	N-CA-C	-6.85	103.65	110.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	118	GLU	Peptide
1	D	89	GLU	Peptide
1	H	93	GLY	Peptide
1	I	30	LYS	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	1520	0	1514	70	0
1	B	1524	0	1514	84	0
1	C	1498	0	1474	90	0
1	D	1496	0	1499	89	0
1	E	1493	0	1465	85	0
1	F	1480	0	1448	110	0
1	G	1501	0	1487	80	0
1	H	1514	0	1503	87	0
1	I	1497	0	1476	81	0
1	J	1506	0	1488	87	0
2	B	8	0	10	0	0
2	E	8	0	10	2	0
2	G	8	0	10	3	0
2	H	8	0	10	1	0
2	J	8	0	10	0	0
3	C	8	0	10	1	0
4	A	48	0	0	1	0
4	B	52	0	0	0	0
4	C	27	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	32	0	0	4	0
4	E	20	0	0	3	0
4	F	33	0	0	4	0
4	G	48	0	0	3	0
4	H	39	0	0	3	0
4	I	30	0	0	3	0
4	J	23	0	0	3	0
All	All	15429	0	14928	772	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 26.

The worst 5 of 772 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:73:THR:HG21	1:B:119:GLY:O	1.51	1.07
1:D:136:HIS:NE2	1:D:138:THR:HG22	1.71	1.06
1:C:180:LYS:HD2	1:C:185:ASP:HB3	1.39	1.05
1:I:24:VAL:HG21	1:I:100:LEU:HD22	1.41	1.03
1:G:46:VAL:HG12	1:H:167:VAL:CG1	1.88	1.03

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	194/216 (90%)	179 (92%)	13 (7%)	2 (1%)	12 38
1	B	196/216 (91%)	180 (92%)	15 (8%)	1 (0%)	24 55
1	C	194/216 (90%)	171 (88%)	23 (12%)	0	100 100
1	D	192/216 (89%)	175 (91%)	15 (8%)	2 (1%)	12 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	193/216 (89%)	173 (90%)	18 (9%)	2 (1%)	12	38
1	F	192/216 (89%)	168 (88%)	22 (12%)	2 (1%)	12	38
1	G	193/216 (89%)	176 (91%)	16 (8%)	1 (0%)	24	55
1	H	194/216 (90%)	171 (88%)	21 (11%)	2 (1%)	12	38
1	I	193/216 (89%)	178 (92%)	15 (8%)	0	100	100
1	J	194/216 (90%)	177 (91%)	16 (8%)	1 (0%)	24	55
All	All	1935/2160 (90%)	1748 (90%)	174 (9%)	13 (1%)	18	47

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	88	LYS
1	G	40	PRO
1	H	116	GLU
1	D	161	THR
1	E	153	ARG

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	162/181 (90%)	139 (86%)	23 (14%)	3	12
1	B	161/181 (89%)	140 (87%)	21 (13%)	4	14
1	C	157/181 (87%)	127 (81%)	30 (19%)	1	5
1	D	159/181 (88%)	134 (84%)	25 (16%)	2	9
1	E	157/181 (87%)	135 (86%)	22 (14%)	3	12
1	F	155/181 (86%)	133 (86%)	22 (14%)	3	12
1	G	159/181 (88%)	139 (87%)	20 (13%)	4	15
1	H	161/181 (89%)	128 (80%)	33 (20%)	1	4
1	I	158/181 (87%)	128 (81%)	30 (19%)	1	5
1	J	159/181 (88%)	133 (84%)	26 (16%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1588/1810 (88%)	1336 (84%)	252 (16%)	2 9

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	148	VAL
1	I	153	ARG
1	G	12	LYS
1	I	144	VAL
1	J	73	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	147	ASN
1	I	64	GLN
1	G	194	ASN
1	H	159	GLN
1	I	164	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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	DTV	C	201	-	7,7,7	0.73	0	4,8,8	0.56	0
2	DTU	H	201	-	7,7,7	0.84	0	4,8,8	1.57	1 (25%)
2	DTU	E	201	-	7,7,7	0.60	0	4,8,8	1.41	1 (25%)
2	DTU	B	201	-	7,7,7	0.53	0	4,8,8	1.02	0
2	DTU	G	201	-	7,7,7	0.64	0	4,8,8	0.77	0
2	DTU	J	201	-	7,7,7	0.66	0	4,8,8	0.44	0

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	DTV	C	201	-	-	4/8/8/8	-
2	DTU	H	201	-	-	6/8/8/8	-
2	DTU	E	201	-	-	5/8/8/8	-
2	DTU	B	201	-	-	6/8/8/8	-
2	DTU	G	201	-	-	2/8/8/8	-
2	DTU	J	201	-	-	8/8/8/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	DTU	O2-C2-C3	2.26	114.32	109.57
2	E	201	DTU	C3-C4-S4	-2.14	108.45	114.43

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	DTU	C1-C2-C3-O3
2	B	201	DTU	C1-C2-C3-C4
2	B	201	DTU	O2-C2-C3-O3
2	B	201	DTU	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	B	201	DTU	C2-C3-C4-S4

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	201	DTV	1	0
2	H	201	DTU	1	0
2	E	201	DTU	2	0
2	G	201	DTU	3	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 [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, 95th 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 ²)	Q<0.9
1	A	195/216 (90%)	-0.63	0 100 100	2, 10, 25, 44	1 (0%)
1	B	197/216 (91%)	-0.57	0 100 100	3, 11, 25, 42	1 (0%)
1	C	196/216 (90%)	-0.46	1 (0%) 87 82	4, 12, 26, 44	0
1	D	194/216 (89%)	-0.62	0 100 100	5, 13, 24, 40	0
1	E	195/216 (90%)	-0.36	1 (0%) 87 82	4, 11, 23, 48	0
1	F	194/216 (89%)	-0.53	0 100 100	6, 13, 25, 39	0
1	G	195/216 (90%)	-0.61	0 100 100	3, 11, 25, 46	0
1	H	195/216 (90%)	-0.53	0 100 100	4, 12, 24, 44	1 (0%)
1	I	195/216 (90%)	-0.60	0 100 100	4, 11, 25, 44	0
1	J	195/216 (90%)	-0.49	0 100 100	4, 12, 23, 45	1 (0%)
All	All	1951/2160 (90%)	-0.54	2 (0%) 92 90	2, 12, 25, 48	4 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	VAL	2.1
1	C	0	MET	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DTU	E	201	8/8	0.84	0.17	49,57,63,70	0
2	DTU	B	201	8/8	0.85	0.15	47,51,54,58	0
3	DTV	C	201	8/8	0.86	0.17	56,59,63,67	0
2	DTU	H	201	8/8	0.87	0.16	45,53,58,64	0
2	DTU	G	201	8/8	0.88	0.14	55,58,62,66	0
2	DTU	J	201	8/8	0.91	0.14	57,59,64,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.