



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:05 PM UTC

PDB ID : 5EPT / pdb_00005ept
Title : Crystal Structure of *S. cerevisiae* TSA2 in the disulfide state
Authors : Nielsen, M.H.; Kidmose, R.T.; Jenner, L.B.
Deposited on : 2015-11-12
Resolution : 5.00 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
Xtriage (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

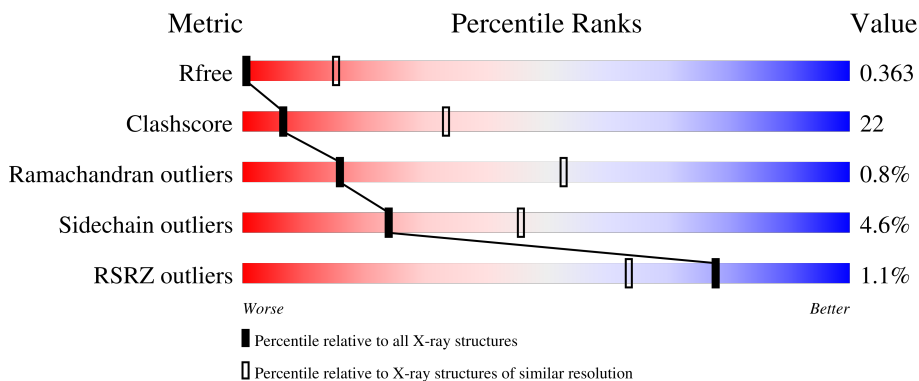
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 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.



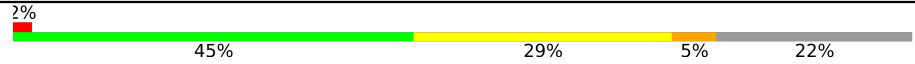

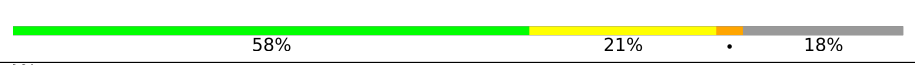

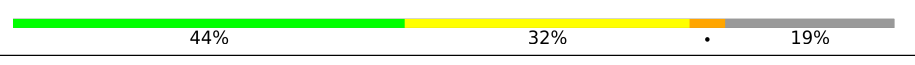
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (6.02-3.98)
Clashscore	190562	1040 (6.00-4.00)
Ramachandran outliers	187476	1015 (6.06-3.92)
Sidechain outliers	187428	1136 (6.10-3.90)
RSRZ outliers	180081	1004 (6.02-3.98)

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	217	 45% 31% 19% 2%
1	B	217	 52% 24% 20% 2%
1	C	217	 56% 22% 21%
1	D	217	 50% 26% 22%
1	E	217	 50% 30% 18%

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Mol	Chain	Length	Quality of chain
1	F	217	 <p>2% 45% 29% 5% 22%</p>
1	G	217	 <p>1% 51% 27% 19%</p>
1	H	217	 <p>0% 58% 21% 18%</p>
1	I	217	 <p>2% 55% 24% 18%</p>
1	J	217	 <p>0% 44% 32% 19%</p>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 13616 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 TSA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	178	1394	906	230	255	3	0	0	0
1	B	173	1342	869	223	247	3	0	0	0
1	C	172	1344	873	222	247	2	0	0	0
1	A	175	1365	887	225	250	3	0	0	0
1	G	175	1365	887	225	250	3	0	0	0
1	I	177	1387	902	229	253	3	0	0	0
1	D	170	1330	864	220	244	2	0	0	0
1	E	178	1394	906	230	255	3	0	0	0
1	J	175	1365	887	225	250	3	0	0	0
1	F	170	1330	864	220	244	2	0	0	0

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-20	MET	-	initiating methionine	UNP Q04120
H	-19	ALA	-	expression tag	UNP Q04120
H	-18	HIS	-	expression tag	UNP Q04120
H	-17	HIS	-	expression tag	UNP Q04120
H	-16	HIS	-	expression tag	UNP Q04120
H	-15	HIS	-	expression tag	UNP Q04120
H	-14	HIS	-	expression tag	UNP Q04120
H	-13	HIS	-	expression tag	UNP Q04120
H	-12	VAL	-	expression tag	UNP Q04120

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	ASP	-	expression tag	UNP Q04120
H	-10	ASP	-	expression tag	UNP Q04120
H	-9	ASP	-	expression tag	UNP Q04120
H	-8	ASP	-	expression tag	UNP Q04120
H	-7	LYS	-	expression tag	UNP Q04120
H	-6	GLU	-	expression tag	UNP Q04120
H	-5	ASN	-	expression tag	UNP Q04120
H	-4	LEU	-	expression tag	UNP Q04120
H	-3	TYR	-	expression tag	UNP Q04120
H	-2	PHE	-	expression tag	UNP Q04120
H	-1	GLN	-	expression tag	UNP Q04120
H	0	GLY	-	expression tag	UNP Q04120
B	-20	MET	-	initiating methionine	UNP Q04120
B	-19	ALA	-	expression tag	UNP Q04120
B	-18	HIS	-	expression tag	UNP Q04120
B	-17	HIS	-	expression tag	UNP Q04120
B	-16	HIS	-	expression tag	UNP Q04120
B	-15	HIS	-	expression tag	UNP Q04120
B	-14	HIS	-	expression tag	UNP Q04120
B	-13	HIS	-	expression tag	UNP Q04120
B	-12	VAL	-	expression tag	UNP Q04120
B	-11	ASP	-	expression tag	UNP Q04120
B	-10	ASP	-	expression tag	UNP Q04120
B	-9	ASP	-	expression tag	UNP Q04120
B	-8	ASP	-	expression tag	UNP Q04120
B	-7	LYS	-	expression tag	UNP Q04120
B	-6	GLU	-	expression tag	UNP Q04120
B	-5	ASN	-	expression tag	UNP Q04120
B	-4	LEU	-	expression tag	UNP Q04120
B	-3	TYR	-	expression tag	UNP Q04120
B	-2	PHE	-	expression tag	UNP Q04120
B	-1	GLN	-	expression tag	UNP Q04120
B	0	GLY	-	expression tag	UNP Q04120
C	-20	MET	-	initiating methionine	UNP Q04120
C	-19	ALA	-	expression tag	UNP Q04120
C	-18	HIS	-	expression tag	UNP Q04120
C	-17	HIS	-	expression tag	UNP Q04120
C	-16	HIS	-	expression tag	UNP Q04120
C	-15	HIS	-	expression tag	UNP Q04120
C	-14	HIS	-	expression tag	UNP Q04120
C	-13	HIS	-	expression tag	UNP Q04120
C	-12	VAL	-	expression tag	UNP Q04120

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	ASP	-	expression tag	UNP Q04120
C	-10	ASP	-	expression tag	UNP Q04120
C	-9	ASP	-	expression tag	UNP Q04120
C	-8	ASP	-	expression tag	UNP Q04120
C	-7	LYS	-	expression tag	UNP Q04120
C	-6	GLU	-	expression tag	UNP Q04120
C	-5	ASN	-	expression tag	UNP Q04120
C	-4	LEU	-	expression tag	UNP Q04120
C	-3	TYR	-	expression tag	UNP Q04120
C	-2	PHE	-	expression tag	UNP Q04120
C	-1	GLN	-	expression tag	UNP Q04120
C	0	GLY	-	expression tag	UNP Q04120
A	-20	MET	-	initiating methionine	UNP Q04120
A	-19	ALA	-	expression tag	UNP Q04120
A	-18	HIS	-	expression tag	UNP Q04120
A	-17	HIS	-	expression tag	UNP Q04120
A	-16	HIS	-	expression tag	UNP Q04120
A	-15	HIS	-	expression tag	UNP Q04120
A	-14	HIS	-	expression tag	UNP Q04120
A	-13	HIS	-	expression tag	UNP Q04120
A	-12	VAL	-	expression tag	UNP Q04120
A	-11	ASP	-	expression tag	UNP Q04120
A	-10	ASP	-	expression tag	UNP Q04120
A	-9	ASP	-	expression tag	UNP Q04120
A	-8	ASP	-	expression tag	UNP Q04120
A	-7	LYS	-	expression tag	UNP Q04120
A	-6	GLU	-	expression tag	UNP Q04120
A	-5	ASN	-	expression tag	UNP Q04120
A	-4	LEU	-	expression tag	UNP Q04120
A	-3	TYR	-	expression tag	UNP Q04120
A	-2	PHE	-	expression tag	UNP Q04120
A	-1	GLN	-	expression tag	UNP Q04120
A	0	GLY	-	expression tag	UNP Q04120
G	-20	MET	-	initiating methionine	UNP Q04120
G	-19	ALA	-	expression tag	UNP Q04120
G	-18	HIS	-	expression tag	UNP Q04120
G	-17	HIS	-	expression tag	UNP Q04120
G	-16	HIS	-	expression tag	UNP Q04120
G	-15	HIS	-	expression tag	UNP Q04120
G	-14	HIS	-	expression tag	UNP Q04120
G	-13	HIS	-	expression tag	UNP Q04120
G	-12	VAL	-	expression tag	UNP Q04120

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-11	ASP	-	expression tag	UNP Q04120
G	-10	ASP	-	expression tag	UNP Q04120
G	-9	ASP	-	expression tag	UNP Q04120
G	-8	ASP	-	expression tag	UNP Q04120
G	-7	LYS	-	expression tag	UNP Q04120
G	-6	GLU	-	expression tag	UNP Q04120
G	-5	ASN	-	expression tag	UNP Q04120
G	-4	LEU	-	expression tag	UNP Q04120
G	-3	TYR	-	expression tag	UNP Q04120
G	-2	PHE	-	expression tag	UNP Q04120
G	-1	GLN	-	expression tag	UNP Q04120
G	0	GLY	-	expression tag	UNP Q04120
I	-20	MET	-	initiating methionine	UNP Q04120
I	-19	ALA	-	expression tag	UNP Q04120
I	-18	HIS	-	expression tag	UNP Q04120
I	-17	HIS	-	expression tag	UNP Q04120
I	-16	HIS	-	expression tag	UNP Q04120
I	-15	HIS	-	expression tag	UNP Q04120
I	-14	HIS	-	expression tag	UNP Q04120
I	-13	HIS	-	expression tag	UNP Q04120
I	-12	VAL	-	expression tag	UNP Q04120
I	-11	ASP	-	expression tag	UNP Q04120
I	-10	ASP	-	expression tag	UNP Q04120
I	-9	ASP	-	expression tag	UNP Q04120
I	-8	ASP	-	expression tag	UNP Q04120
I	-7	LYS	-	expression tag	UNP Q04120
I	-6	GLU	-	expression tag	UNP Q04120
I	-5	ASN	-	expression tag	UNP Q04120
I	-4	LEU	-	expression tag	UNP Q04120
I	-3	TYR	-	expression tag	UNP Q04120
I	-2	PHE	-	expression tag	UNP Q04120
I	-1	GLN	-	expression tag	UNP Q04120
I	0	GLY	-	expression tag	UNP Q04120
D	-20	MET	-	initiating methionine	UNP Q04120
D	-19	ALA	-	expression tag	UNP Q04120
D	-18	HIS	-	expression tag	UNP Q04120
D	-17	HIS	-	expression tag	UNP Q04120
D	-16	HIS	-	expression tag	UNP Q04120
D	-15	HIS	-	expression tag	UNP Q04120
D	-14	HIS	-	expression tag	UNP Q04120
D	-13	HIS	-	expression tag	UNP Q04120
D	-12	VAL	-	expression tag	UNP Q04120

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	ASP	-	expression tag	UNP Q04120
D	-10	ASP	-	expression tag	UNP Q04120
D	-9	ASP	-	expression tag	UNP Q04120
D	-8	ASP	-	expression tag	UNP Q04120
D	-7	LYS	-	expression tag	UNP Q04120
D	-6	GLU	-	expression tag	UNP Q04120
D	-5	ASN	-	expression tag	UNP Q04120
D	-4	LEU	-	expression tag	UNP Q04120
D	-3	TYR	-	expression tag	UNP Q04120
D	-2	PHE	-	expression tag	UNP Q04120
D	-1	GLN	-	expression tag	UNP Q04120
D	0	GLY	-	expression tag	UNP Q04120
E	-20	MET	-	initiating methionine	UNP Q04120
E	-19	ALA	-	expression tag	UNP Q04120
E	-18	HIS	-	expression tag	UNP Q04120
E	-17	HIS	-	expression tag	UNP Q04120
E	-16	HIS	-	expression tag	UNP Q04120
E	-15	HIS	-	expression tag	UNP Q04120
E	-14	HIS	-	expression tag	UNP Q04120
E	-13	HIS	-	expression tag	UNP Q04120
E	-12	VAL	-	expression tag	UNP Q04120
E	-11	ASP	-	expression tag	UNP Q04120
E	-10	ASP	-	expression tag	UNP Q04120
E	-9	ASP	-	expression tag	UNP Q04120
E	-8	ASP	-	expression tag	UNP Q04120
E	-7	LYS	-	expression tag	UNP Q04120
E	-6	GLU	-	expression tag	UNP Q04120
E	-5	ASN	-	expression tag	UNP Q04120
E	-4	LEU	-	expression tag	UNP Q04120
E	-3	TYR	-	expression tag	UNP Q04120
E	-2	PHE	-	expression tag	UNP Q04120
E	-1	GLN	-	expression tag	UNP Q04120
E	0	GLY	-	expression tag	UNP Q04120
J	-20	MET	-	initiating methionine	UNP Q04120
J	-19	ALA	-	expression tag	UNP Q04120
J	-18	HIS	-	expression tag	UNP Q04120
J	-17	HIS	-	expression tag	UNP Q04120
J	-16	HIS	-	expression tag	UNP Q04120
J	-15	HIS	-	expression tag	UNP Q04120
J	-14	HIS	-	expression tag	UNP Q04120
J	-13	HIS	-	expression tag	UNP Q04120
J	-12	VAL	-	expression tag	UNP Q04120

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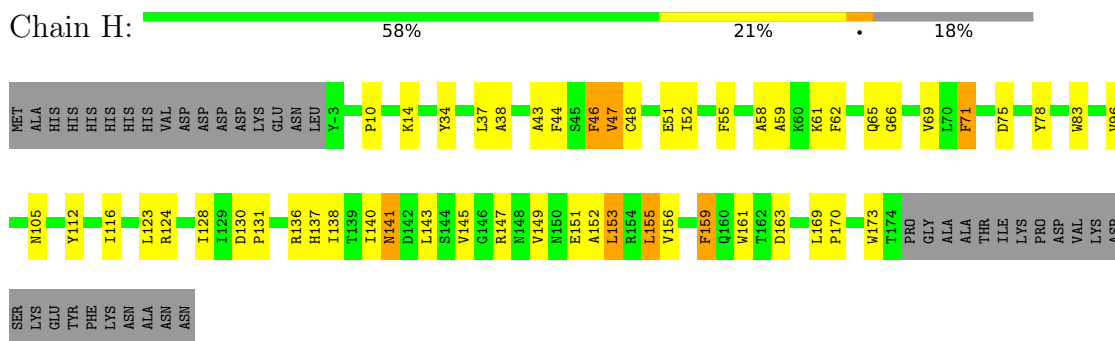
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Chain	Residue	Modelled	Actual	Comment	Reference
J	-11	ASP	-	expression tag	UNP Q04120
J	-10	ASP	-	expression tag	UNP Q04120
J	-9	ASP	-	expression tag	UNP Q04120
J	-8	ASP	-	expression tag	UNP Q04120
J	-7	LYS	-	expression tag	UNP Q04120
J	-6	GLU	-	expression tag	UNP Q04120
J	-5	ASN	-	expression tag	UNP Q04120
J	-4	LEU	-	expression tag	UNP Q04120
J	-3	TYR	-	expression tag	UNP Q04120
J	-2	PHE	-	expression tag	UNP Q04120
J	-1	GLN	-	expression tag	UNP Q04120
J	0	GLY	-	expression tag	UNP Q04120
F	-20	MET	-	initiating methionine	UNP Q04120
F	-19	ALA	-	expression tag	UNP Q04120
F	-18	HIS	-	expression tag	UNP Q04120
F	-17	HIS	-	expression tag	UNP Q04120
F	-16	HIS	-	expression tag	UNP Q04120
F	-15	HIS	-	expression tag	UNP Q04120
F	-14	HIS	-	expression tag	UNP Q04120
F	-13	HIS	-	expression tag	UNP Q04120
F	-12	VAL	-	expression tag	UNP Q04120
F	-11	ASP	-	expression tag	UNP Q04120
F	-10	ASP	-	expression tag	UNP Q04120
F	-9	ASP	-	expression tag	UNP Q04120
F	-8	ASP	-	expression tag	UNP Q04120
F	-7	LYS	-	expression tag	UNP Q04120
F	-6	GLU	-	expression tag	UNP Q04120
F	-5	ASN	-	expression tag	UNP Q04120
F	-4	LEU	-	expression tag	UNP Q04120
F	-3	TYR	-	expression tag	UNP Q04120
F	-2	PHE	-	expression tag	UNP Q04120
F	-1	GLN	-	expression tag	UNP Q04120
F	0	GLY	-	expression tag	UNP Q04120

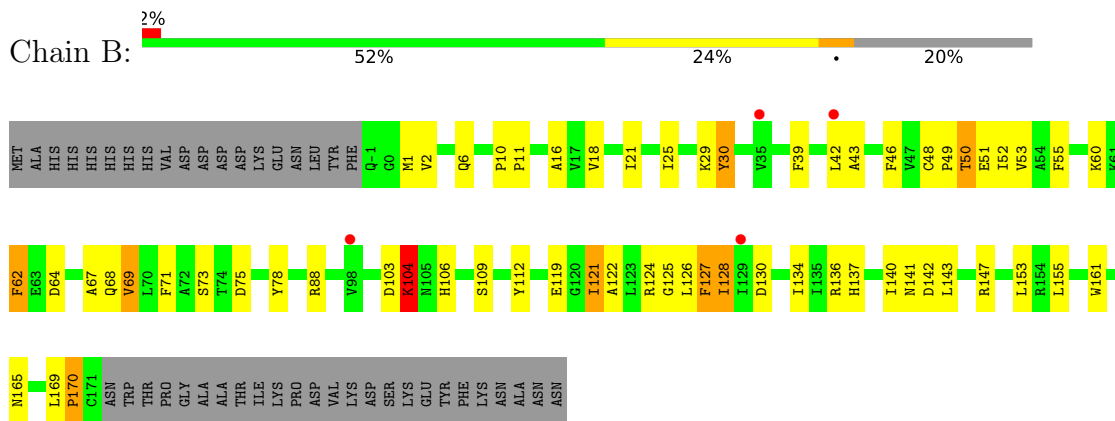
3 Residue-property plots [i](#)

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.

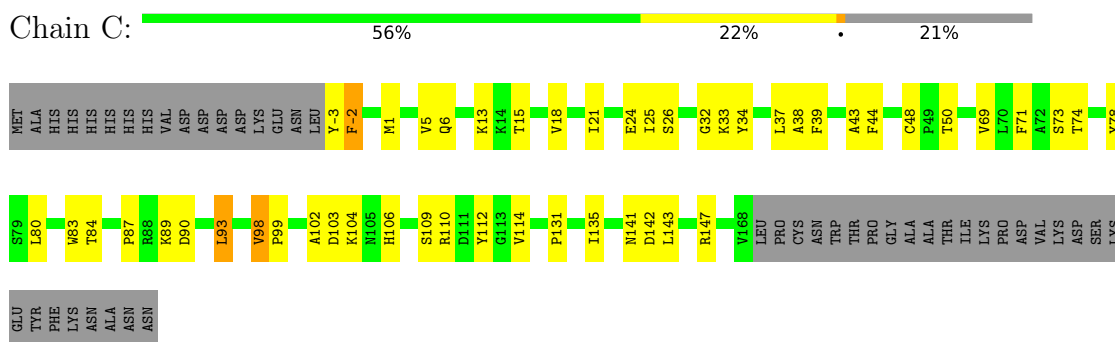
• Molecule 1: Peroxiredoxin TSA2



• Molecule 1: Peroxiredoxin TSA2



• Molecule 1: Peroxiredoxin TSA2



THR
PRO
GLY
ALA
ALA
THR
ILE
LYS
PRO
VAL
ASP
VAL
LYS
ASP
SER
LYS
GLU
GLU
ASN
LEU
PHE
PHE
LYS
ASN
ALA
ASN

• Molecule 1: Peroxiredoxin TSA2

Chain E: 50% 30% 18%

MET
ALA
HIS
HIS
HIS
HIS
HIS
HIS
VAL
ASP
ASP
ASP
ASP
LYS
GLU
GLU
ASN
LEU
Y-3
F-2
Q-1
V5
A9
P10
K14
T15
A16
F22
I25
E28
K29
Y30
K31
Y34
L37
A38
F39
L42
A43
F44
S45
F46
V47
C48
P49
T50
E51
I52
F55
K61

Q65
Q68
L70
F71
A72
S73
T74
Y78
W83
R88
G92
L93
L100
D103
K104
M105
H106
S107
Y112
G113
V114
R124
G125
L126
F127
I128
I129
D130
P131
K132
G133
I134
I135
R136
H137
N141
D142
L143
S144
E145
S144
R147
T50
N148
V149
A152
L153

V156
Q160
D163
P170
I174
PRO
GLY
ALA
ALA
THR
ILE
LYS
ASN
PRO
LEU
VAL
ASP
LYS
ASP
LYS
SER
LYS
GLU
GLU
THR
PHE
LYS
ASN
ASN
ASN

• Molecule 1: Peroxiredoxin TSA2

Chain J: 44% 32% 19%

MET
ALA
HIS
HIS
HIS
HIS
HIS
VAL
ASP
ASP
ASP
ASP
LYS
GLU
GLU
ASN
LEU
Y-3
F-2
M1
V2
A3
F4
V5
Q6
A9
V18
E22
E23
K29
Y34
V35
V36
L37
A38
V40
A43
C48
P49
A53
A59
F62
Q65
V69
S73
T74

D75
S76
E77
Y78
R88
G92
R97
V98
P99
A102
D103
K104
M105
H106
S107
L108
S109
R110
D111
Y112
G113
V114
E117
I121
R124
G125
F127
I128
I129
D130
P131
I135
R136
H137
I138
I139
M140
D142
L143
S144
E145
G146
R147
M148
V149
L155
V156
E157
G158

F159
Q160
M161
T162
D163
M164
W165
G166
T167
V168
L169
P170
C171
ASN
TRP
THR
PRO
GLY
ALA
ALA
THR
ILE
LYS
PRO
ASP
VAL
LYS
ASP
SER
LYS
GLU
TYR
PHE
LYS
ASN
ALA
ASN
ASN

• Molecule 1: Peroxiredoxin TSA2

Chain F: 2% 45% 29% 5% 22%

MET
ALA
HIS
HIS
HIS
HIS
HIS
VAL
ASP
ASP
ASP
ASP
LYS
GLU
GLU
ASN
LEU
Y-3
F-2
M1
V2
V5
F6
Q8
F12
K13
K14
T15
A16
G20
S26
Y34
V35
V36
L37
A38
F39
A43
C48
P49
T50
E51
I52
V53
A54
F55
F62
A67
Q68

V69
L70
F71
T74
D75
S76
E77
Y78
L80
H83
L86
P87
L93
Y96
L100
L101
A102
D103
L108
D111
Y112
A122
L123
G125
L126
F127
I128
D129
P131
K132
G133
I134
I135
R136
H137
D142
L143
S144
V145
G146
R147
N148
V149
M150
E151
A152
L153

R154
L155
F159
T162
D163
K164
M165
G166
THR
VAL
LEU
PRO
CYS
ASN
TRP
THR
PRO
GLY
ALA
THR
ILE
LYS
PRO
ASP
VAL
LYS
SER
LYS
GLU
TYR
PHE
LYS
ASN
ALA
ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.46Å 167.21Å 221.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.35 – 5.00 46.35 – 5.00	Depositor EDS
% Data completeness (in resolution range)	83.2 (46.35-5.00) 78.0 (46.35-5.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.64 (at 4.00Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.274 , 0.375 0.282 , 0.363	Depositor DCC
R_{free} test set	1348 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	132.4	Xtrriage
Anisotropy	1.259	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 394.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13616	wwPDB-VP
Average B, all atoms (Å ²)	350.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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

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	0.32	1/1395 (0.1%)	0.67	0/1890
1	B	0.26	0/1370	0.56	0/1856
1	C	0.25	0/1373	0.59	0/1859
1	D	0.31	0/1359	0.60	0/1839
1	E	0.27	0/1426	0.67	0/1934
1	F	0.22	0/1359	0.63	0/1839
1	G	0.29	0/1395	0.62	0/1890
1	H	0.24	0/1426	0.58	0/1934
1	I	0.25	0/1419	0.56	1/1924 (0.1%)
1	J	0.23	0/1395	0.65	0/1890
All	All	0.27	1/13917 (0.0%)	0.62	1/18855 (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	A	0	1
1	B	0	1
1	I	0	1
1	J	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	A	8	GLN	CD-OE1	6.33	1.35	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	154	ARG	CB-CG-CD	5.04	122.88	111.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	GLN	Sidechain
1	B	50	THR	Peptide
1	I	-2	PHE	Peptide
1	J	140	ILE	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	1365	0	1388	78	0
1	B	1342	0	1370	64	0
1	C	1344	0	1367	36	0
1	D	1330	0	1351	66	0
1	E	1394	0	1412	67	0
1	F	1330	0	1350	78	0
1	G	1365	0	1388	72	0
1	H	1394	0	1411	52	0
1	I	1387	0	1404	55	0
1	J	1365	0	1388	79	0
All	All	13616	0	13829	591	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 22.

The worst 5 of 591 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:H:170:PRO:C	1:G:48:CYS:SG	2.41	1.04
1:B:125:GLY:O	1:B:147:ARG:NH1	1.94	1.01
1:B:169:LEU:O	1:B:170:PRO:O	1.76	1.01
1:G:46:PHE:HE2	1:F:78:TYR:CE1	1.78	1.01
1:D:86:LEU:HG	1:D:91:GLY:HA2	1.41	0.99

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	173/217 (80%)	161 (93%)	11 (6%)	1 (1%)	21	58
1	B	171/217 (79%)	161 (94%)	7 (4%)	3 (2%)	6	32
1	C	170/217 (78%)	160 (94%)	10 (6%)	0	100	100
1	D	168/217 (77%)	155 (92%)	13 (8%)	0	100	100
1	E	176/217 (81%)	167 (95%)	9 (5%)	0	100	100
1	F	168/217 (77%)	156 (93%)	11 (6%)	1 (1%)	21	58
1	G	173/217 (80%)	162 (94%)	9 (5%)	2 (1%)	10	42
1	H	176/217 (81%)	166 (94%)	9 (5%)	1 (1%)	21	58
1	I	175/217 (81%)	164 (94%)	10 (6%)	1 (1%)	21	58
1	J	173/217 (80%)	153 (88%)	16 (9%)	4 (2%)	5	27
All	All	1723/2170 (79%)	1605 (93%)	105 (6%)	13 (1%)	16	53

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	PRO
1	A	47	VAL
1	G	3	ALA
1	J	141	ASN
1	B	104	LYS

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	147/184 (80%)	136 (92%)	11 (8%)	12	33
1	B	145/184 (79%)	137 (94%)	8 (6%)	19	42
1	C	144/184 (78%)	140 (97%)	4 (3%)	38	59
1	D	142/184 (77%)	135 (95%)	7 (5%)	22	44
1	E	150/184 (82%)	146 (97%)	4 (3%)	39	60
1	F	142/184 (77%)	132 (93%)	10 (7%)	14	36
1	G	147/184 (80%)	142 (97%)	5 (3%)	32	54
1	H	150/184 (82%)	142 (95%)	8 (5%)	20	42
1	I	149/184 (81%)	145 (97%)	4 (3%)	39	60
1	J	147/184 (80%)	141 (96%)	6 (4%)	27	49
All	All	1463/1840 (80%)	1396 (95%)	67 (5%)	24	46

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	-2	PHE
1	F	34	TYR
1	F	149	VAL
1	A	35	VAL
1	A	34	TYR

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

Mol	Chain	Res	Type
1	E	106	HIS
1	J	85	ASN
1	F	165	ASN
1	F	160	GLN
1	G	141	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](#)

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, 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	175/217 (80%)	-0.20	3 (1%) 69 56	313, 374, 442, 476	0
1	B	173/217 (79%)	-0.05	4 (2%) 61 50	311, 364, 413, 508	0
1	C	172/217 (79%)	-0.41	0 100 100	307, 370, 441, 493	0
1	D	170/217 (78%)	-0.24	1 (0%) 85 73	314, 361, 444, 598	0
1	E	178/217 (82%)	-0.41	0 100 100	302, 350, 391, 445	0
1	F	170/217 (78%)	-0.05	4 (2%) 59 49	266, 319, 375, 482	0
1	G	175/217 (80%)	-0.18	3 (1%) 69 56	239, 304, 378, 411	0
1	H	178/217 (82%)	-0.31	0 100 100	259, 302, 368, 462	0
1	I	177/217 (81%)	-0.35	4 (2%) 61 50	274, 332, 396, 413	0
1	J	175/217 (80%)	-0.29	1 (0%) 85 73	306, 356, 422, 578	0
All	All	1743/2170 (80%)	-0.25	20 (1%) 78 63	239, 348, 416, 598	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	144	SER	5.4
1	F	100	LEU	4.6
1	F	71	PHE	4.4
1	A	72	ALA	3.7
1	B	98	VAL	3.5

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.