



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:02 PM GMT

PDB ID : 3SBC  
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](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

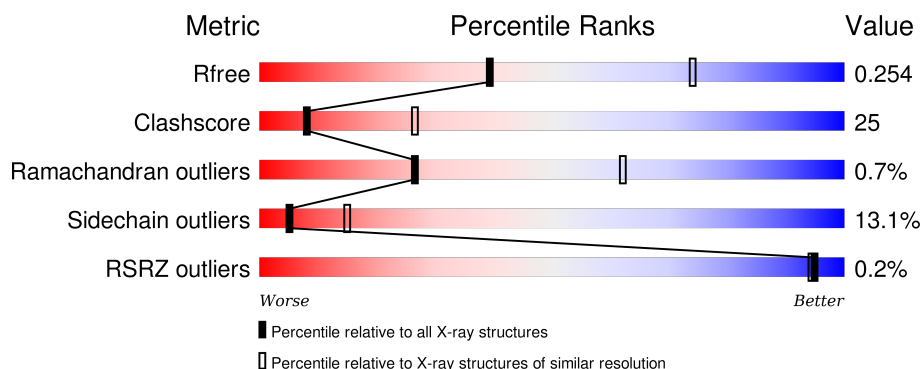
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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	216	<div> <div>58%</div> <div>26%</div> <div>5%</div> <div>10%</div> </div>
1	B	216	<div> <div>50%</div> <div>35%</div> <div>6%</div> <div>9%</div> </div>
1	C	216	<div> <div>42%</div> <div>43%</div> <div>5%</div> <div>9%</div> </div>
1	D	216	<div> <div>44%</div> <div>40%</div> <div>5%</div> <div>10%</div> </div>
1	E	216	<div> <div>49%</div> <div>37%</div> <div>•</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	216	
1	G	216	
1	H	216	
1	I	216	
1	J	216	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DTU	B	201	-	-	-	X
2	DTU	E	201	-	-	-	X
2	DTU	H	201	-	-	-	X
2	DTU	J	201	-	-	-	X

## 2 Entry composition

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

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
C	-13	HIS	-	EXPRESSION TAG	UNP P34760
C	-12	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
D	-8	GLY	-	EXPRESSION TAG	UNP P34760
D	-7	LEU	-	EXPRESSION TAG	UNP P34760
D	-6	VAL	-	EXPRESSION TAG	UNP P34760
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
H	-6	VAL	-	EXPRESSION TAG	UNP P34760
H	-5	PRO	-	EXPRESSION TAG	UNP P34760
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
I	-17	SER	-	EXPRESSION TAG	UNP P34760
I	-16	HIS	-	EXPRESSION TAG	UNP P34760
I	-15	HIS	-	EXPRESSION TAG	UNP P34760
I	-14	HIS	-	EXPRESSION TAG	UNP P34760
I	-13	HIS	-	EXPRESSION TAG	UNP P34760
I	-12	HIS	-	EXPRESSION TAG	UNP P34760

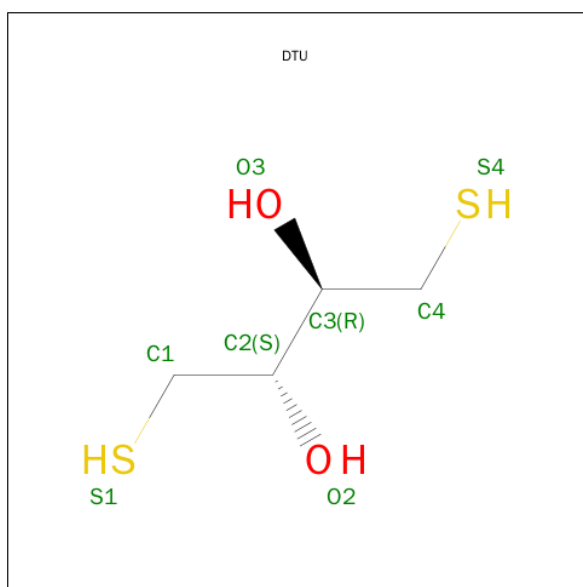
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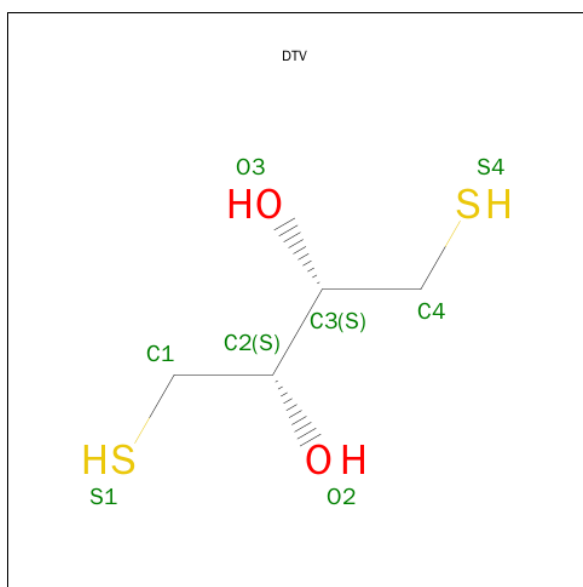
Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	EXPRESSION TAG	UNP P34760
I	-10	SER	-	EXPRESSION TAG	UNP P34760
I	-9	SER	-	EXPRESSION TAG	UNP P34760
I	-8	GLY	-	EXPRESSION TAG	UNP P34760
I	-7	LEU	-	EXPRESSION TAG	UNP P34760
I	-6	VAL	-	EXPRESSION TAG	UNP P34760
I	-5	PRO	-	EXPRESSION TAG	UNP 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 (three-letter code: DTU) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



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 (three-letter code: DTU) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



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

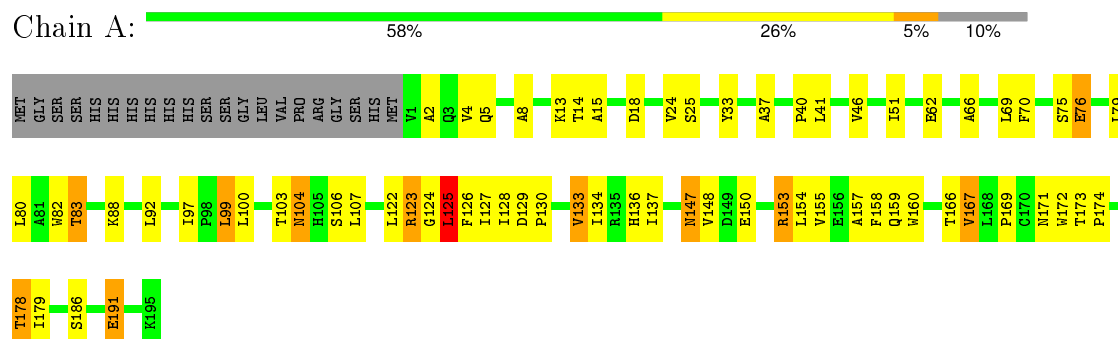
- Molecule 4 is water.

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		

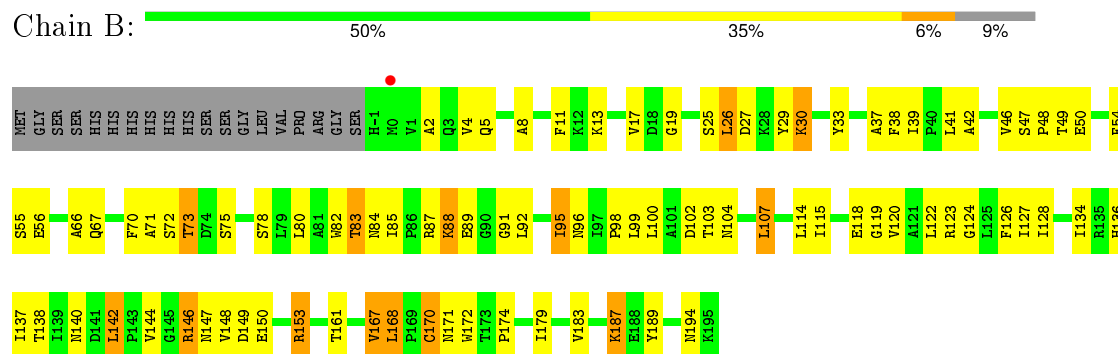
### 3 Residue-property plots

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.

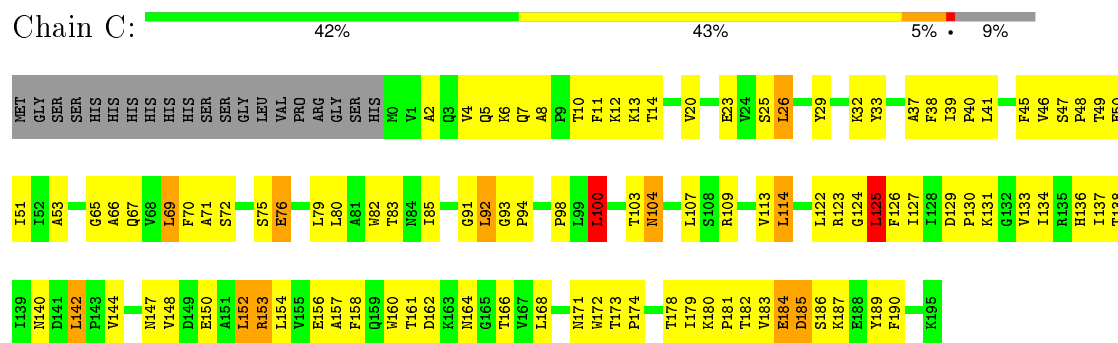
#### • Molecule 1: Peroxiredoxin TSA1



#### • Molecule 1: Peroxiredoxin TSA1

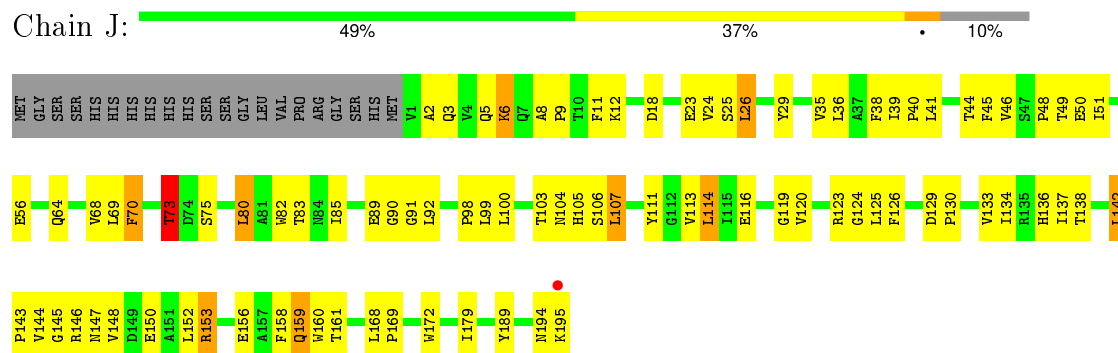


#### • Molecule 1: Peroxiredoxin TSA1



#### • Molecule 1: Peroxiredoxin TSA1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	239.98Å 51.96Å 192.35Å 90.00° 92.33° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 57.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.80) 97.6 (57.90-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.202 , 0.274 0.197 , 0.254	Depositor DCC
$R_{free}$ test set	2933 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 23.4	EDS
Estimated twinning fraction	0.937 for H, K, L 0.063 for -H, -K, L 0.054 for -h,-k,l	Xtriage
Reported twinning fraction	0.937 for H, K, L 0.063 for -H, -K, L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 58039 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15429	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage'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.*

<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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DTV, 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	0.76	0/1554	0.82	1/2117 (0.0%)
1	B	0.78	1/1558 (0.1%)	0.85	1/2123 (0.0%)
1	C	0.73	0/1532	0.83	3/2092 (0.1%)
1	D	0.82	3/1530 (0.2%)	0.91	1/2085 (0.0%)
1	E	0.67	0/1527	0.82	1/2086 (0.0%)
1	F	0.82	0/1514	0.85	0/2070
1	G	0.74	0/1535	0.82	1/2094 (0.0%)
1	H	0.81	0/1548	0.91	3/2110 (0.1%)
1	I	0.71	1/1531 (0.1%)	0.79	1/2090 (0.0%)
1	J	0.80	0/1540	0.86	1/2101 (0.0%)
All	All	0.76	5/15369 (0.0%)	0.85	13/20968 (0.1%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	170	CYS	CB-SG	-6.09	1.71	1.82
1	I	170	CYS	CB-SG	-5.82	1.72	1.81
1	D	56	GLU	CG-CD	5.64	1.60	1.51
1	B	170	CYS	CB-SG	-5.49	1.72	1.81
1	D	89	GLU	CG-CD	5.06	1.59	1.51



The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	153	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	D	91	GLY	N-CA-C	-6.85	95.98	113.10
1	A	125	LEU	CA-CB-CG	6.70	130.72	115.30
1	C	125	LEU	CA-CB-CG	6.65	130.59	115.30
1	H	146	ARG	NE-CZ-NH2	6.15	123.38	120.30

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

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	68	0
1	B	1524	0	1514	78	0
1	C	1498	0	1474	87	0
1	D	1496	0	1499	84	0
1	E	1493	0	1465	80	0
1	F	1480	0	1448	103	0
1	G	1501	0	1487	79	0
1	H	1514	0	1503	85	0
1	I	1497	0	1476	78	0
1	J	1506	0	1488	85	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	52	0	0	0	0
4	C	27	0	0	2	0
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	737	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 25.

The worst 5 of 737 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%)	19	52
1	B	196/216 (91%)	180 (92%)	15 (8%)	1 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	194/216 (90%)	171 (88%)	23 (12%)	0	100	100
1	D	192/216 (89%)	175 (91%)	15 (8%)	2 (1%)	19	52
1	E	193/216 (89%)	173 (90%)	18 (9%)	2 (1%)	19	52
1	F	192/216 (89%)	168 (88%)	22 (12%)	2 (1%)	19	52
1	G	193/216 (89%)	176 (91%)	16 (8%)	1 (0%)	34	69
1	H	194/216 (90%)	171 (88%)	21 (11%)	2 (1%)	19	52
1	I	193/216 (89%)	178 (92%)	15 (8%)	0	100	100
1	J	194/216 (90%)	177 (91%)	16 (8%)	1 (0%)	34	69
All	All	1935/2160 (90%)	1748 (90%)	174 (9%)	13 (1%)	26	62

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 ⓘ

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%)	145 (90%)	17 (10%)	8	24
1	B	161/181 (89%)	143 (89%)	18 (11%)	7	22
1	C	157/181 (87%)	132 (84%)	25 (16%)	3	9
1	D	159/181 (88%)	137 (86%)	22 (14%)	4	13
1	E	157/181 (87%)	140 (89%)	17 (11%)	8	23
1	F	155/181 (86%)	137 (88%)	18 (12%)	7	20
1	G	159/181 (88%)	139 (87%)	20 (13%)	5	17
1	H	161/181 (89%)	135 (84%)	26 (16%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	158/181 (87%)	131 (83%)	27 (17%)	2	7
1	J	159/181 (88%)	142 (89%)	17 (11%)	8	24
All	All	1588/1810 (88%)	1381 (87%)	207 (13%)	5	15

5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	125	LEU
1	F	173	THR
1	J	18	ASP
1	E	152	LEU
1	F	80	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	7	GLN
1	G	105	HIS
1	J	105	HIS
1	G	67	GLN
1	G	96	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](#)

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	$\# Z  > 2$
2	DTU	B	201	-	7,7,7	0.59	0	4,8,8	1.25	0
3	DTV	C	201	-	7,7,7	0.80	0	4,8,8	0.85	0
2	DTU	E	201	-	7,7,7	0.68	0	4,8,8	1.95	1 (25%)
2	DTU	G	201	-	7,7,7	0.66	0	4,8,8	1.01	0
2	DTU	H	201	-	7,7,7	0.87	0	4,8,8	1.66	2 (50%)
2	DTU	J	201	-	7,7,7	0.69	0	4,8,8	0.62	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
2	DTU	B	201	-	-	0/8/8/8	0/0/0/0
3	DTV	C	201	-	-	0/8/8/8	0/0/0/0
2	DTU	E	201	-	-	0/8/8/8	0/0/0/0
2	DTU	G	201	-	-	0/8/8/8	0/0/0/0
2	DTU	H	201	-	-	0/8/8/8	0/0/0/0
2	DTU	J	201	-	-	0/8/8/8	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	DTU	C3-C4-S4	-3.29	108.45	113.91
2	H	201	DTU	O3-C3-C2	-2.13	105.43	109.79
2	H	201	DTU	O2-C2-C3	2.22	114.32	109.79

There are no chirality outliers.

There are no torsion outliers.

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	E	201	DTU	2	0
2	G	201	DTU	3	0
2	H	201	DTU	1	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, 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	195/216 (90%)	-0.29	0 <span>100</span> <span>100</span>	3, 10, 25, 44	0
1	B	197/216 (91%)	-0.16	1 (0%) <span>91</span> <span>88</span>	3, 11, 25, 42	0
1	C	196/216 (90%)	-0.15	0 <span>100</span> <span>100</span>	4, 12, 26, 44	0
1	D	194/216 (89%)	-0.35	0 <span>100</span> <span>100</span>	5, 13, 24, 40	0
1	E	195/216 (90%)	-0.16	2 (1%) <span>84</span> <span>77</span>	4, 11, 23, 48	0
1	F	194/216 (89%)	-0.17	0 <span>100</span> <span>100</span>	6, 13, 25, 39	0
1	G	195/216 (90%)	-0.19	0 <span>100</span> <span>100</span>	3, 11, 25, 46	0
1	H	195/216 (90%)	-0.23	0 <span>100</span> <span>100</span>	4, 12, 24, 44	0
1	I	195/216 (90%)	-0.20	0 <span>100</span> <span>100</span>	4, 11, 25, 44	0
1	J	195/216 (90%)	-0.16	1 (0%) <span>91</span> <span>88</span>	4, 12, 23, 45	0
All	All	1951/2160 (90%)	-0.21	4 (0%) <span>95</span> <span>94</span>	3, 12, 25, 48	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	192	ALA	2.4
1	B	0	MET	2.1
1	J	195	LYS	2.0
1	E	190	PHE	2.0

### 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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DTU	E	201	8/8	0.81	0.28	5.08	49,57,63,70	0
2	DTU	H	201	8/8	0.87	0.25	5.07	45,53,58,64	0
2	DTU	B	201	8/8	0.83	0.23	2.71	47,51,54,58	0
2	DTU	J	201	8/8	0.87	0.27	2.63	57,59,64,68	0
3	DTV	C	201	8/8	0.84	0.23	0.98	56,59,63,67	0
2	DTU	G	201	8/8	0.86	0.22	0.86	55,58,62,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.