



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 07:46 pm BST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

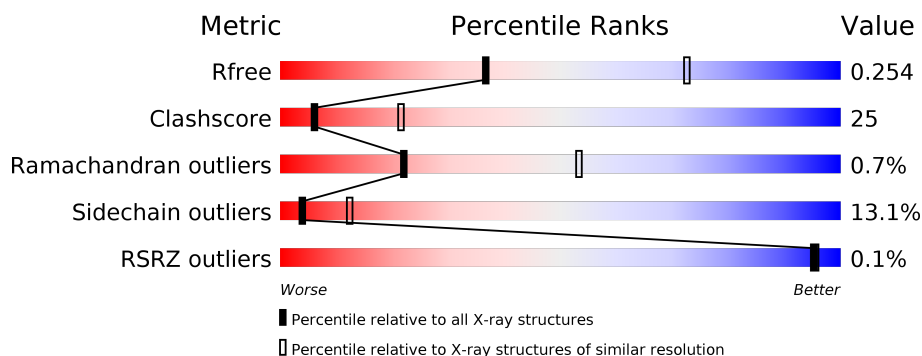
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 ≥ 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	<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>
1	F	216	<div> <div>44%</div> <div>39%</div> <div>7%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	216	<div><div></div><div>50%35%5%10%</div></div>
1	H	216	<div><div></div><div>50%31%9%10%</div></div>
1	I	216	<div><div></div><div>49%35%7%10%</div></div>
1	J	216	<div><div></div><div>49%37%•10%</div></div>

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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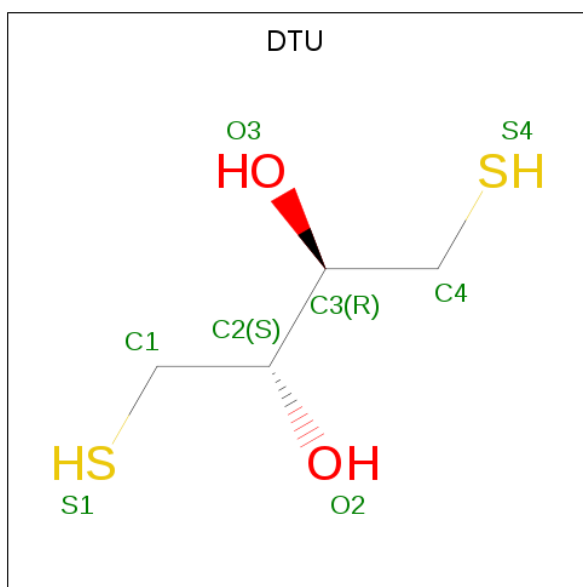
Chain	Residue	Modelled	Actual	Comment	Reference
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G	-10	SER	-	EXPRESSION TAG	UNP P34760
G	-9	SER	-	EXPRESSION TAG	UNP P34760
G	-8	GLY	-	EXPRESSION TAG	UNP P34760
G	-7	LEU	-	EXPRESSION TAG	UNP P34760
G	-6	VAL	-	EXPRESSION TAG	UNP P34760
G	-5	PRO	-	EXPRESSION 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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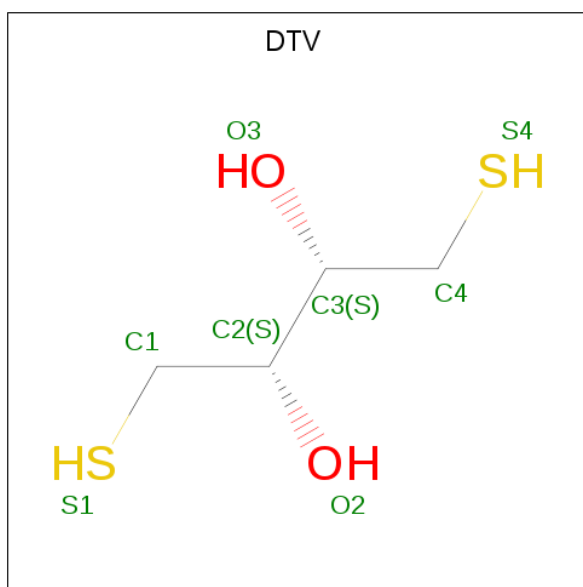
Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	EXPRESSION TAG	UNP P34760
I	-10	SER	-	EXPRESSION TAG	UNP P34760
I	-9	SER	-	EXPRESSION TAG	UNP P34760
I	-8	GLY	-	EXPRESSION TAG	UNP P34760
I	-7	LEU	-	EXPRESSION TAG	UNP P34760
I	-6	VAL	-	EXPRESSION TAG	UNP P34760
I	-5	PRO	-	EXPRESSION TAG	UNP 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: 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 (three-letter code: 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		

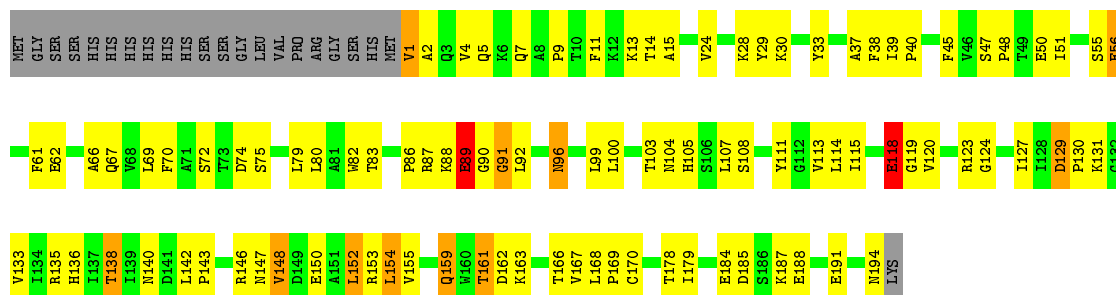
- Molecule 1: Peroxiredoxin TSA1





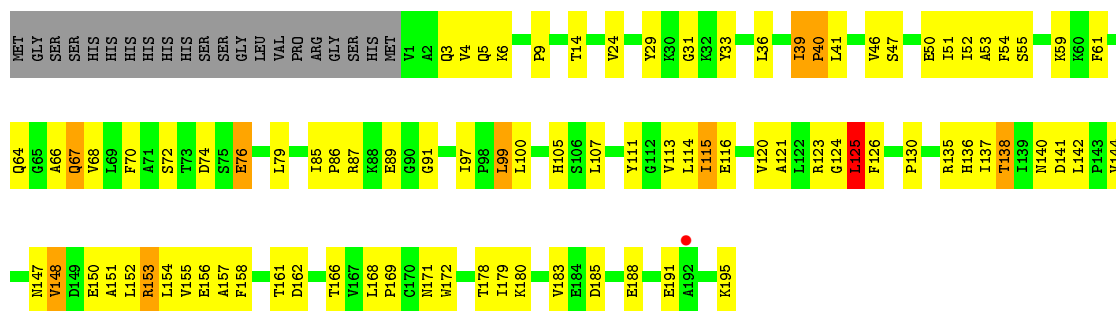
• Molecule 1: Peroxiredoxin TSA1

Chain D: 44% 40% 5% 10%



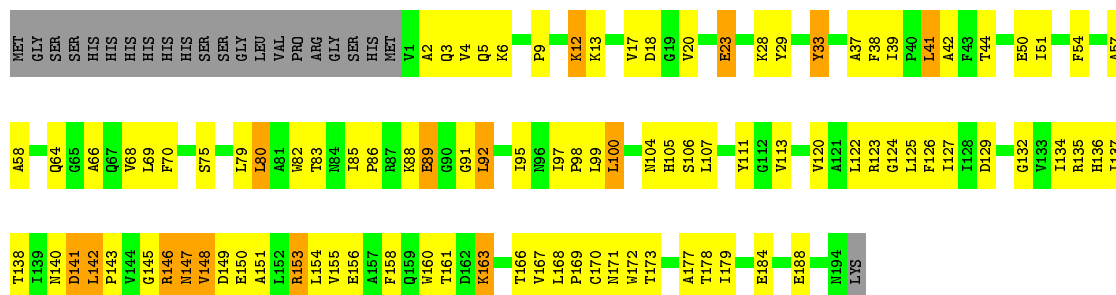
• Molecule 1: Peroxiredoxin TSA1

Chain E: 49% 37% 10%



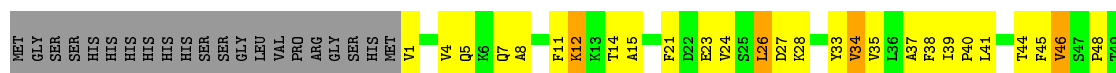
• Molecule 1: Peroxiredoxin TSA1

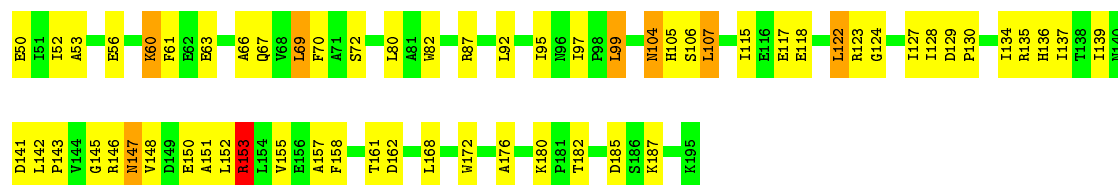
Chain F: 44% 39% 7% 10%



• Molecule 1: Peroxiredoxin TSA1

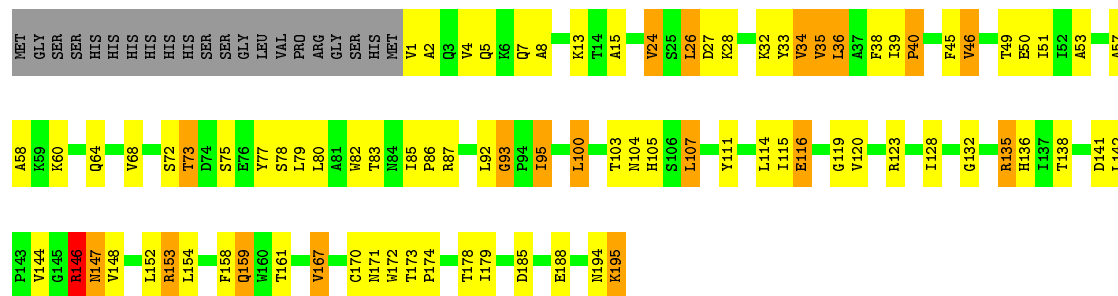
Chain G: 50% 35% 5% 10%





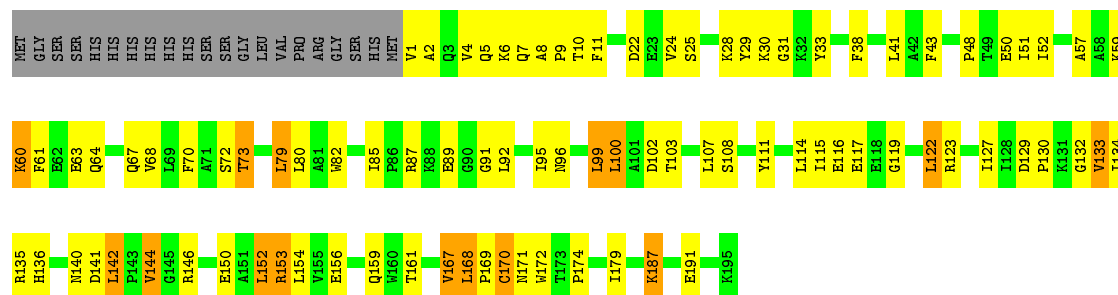
• Molecule 1: Peroxiredoxin TSA1

Chain H: 50% 31% 9% 10%



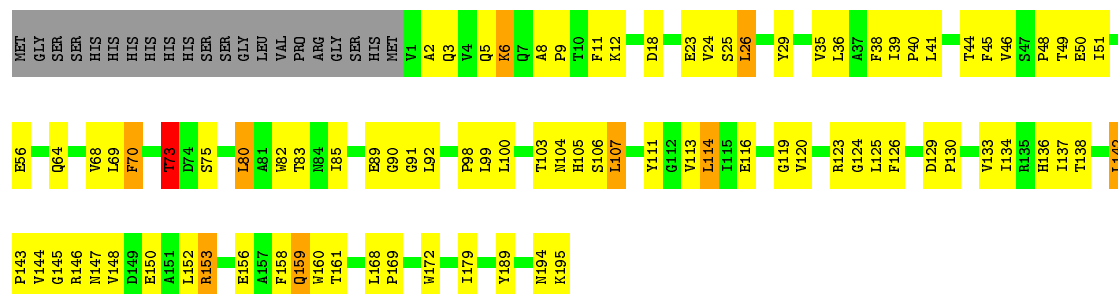
• Molecule 1: Peroxiredoxin TSA1

Chain I: 49% 35% 7% 10%



• Molecule 1: Peroxiredoxin TSA1

Chain J: 49% 37% 10%



4 Data and refinement statistics

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 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
$\langle I/\sigma(I) \rangle$ ¹	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 (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 23.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
Reported twinning fraction	0.937 for H, K, L 0.063 for -h,-k,l	Depositor
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 ²)	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.*

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 ⓘ

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%)	15	44
1	B	196/216 (91%)	180 (92%)	15 (8%)	1 (0%)	29	61

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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%)	15	44
1	E	193/216 (89%)	173 (90%)	18 (9%)	2 (1%)	15	44
1	F	192/216 (89%)	168 (88%)	22 (12%)	2 (1%)	15	44
1	G	193/216 (89%)	176 (91%)	16 (8%)	1 (0%)	29	61
1	H	194/216 (90%)	171 (88%)	21 (11%)	2 (1%)	15	44
1	I	193/216 (89%)	178 (92%)	15 (8%)	0	100	100
1	J	194/216 (90%)	177 (91%)	16 (8%)	1 (0%)	29	61
All	All	1935/2160 (90%)	1748 (90%)	174 (9%)	13 (1%)	22	53

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%)	7	20
1	B	161/181 (89%)	143 (89%)	18 (11%)	6	18
1	C	157/181 (87%)	132 (84%)	25 (16%)	2	7
1	D	159/181 (88%)	137 (86%)	22 (14%)	3	11
1	E	157/181 (87%)	140 (89%)	17 (11%)	6	19
1	F	155/181 (86%)	137 (88%)	18 (12%)	5	17
1	G	159/181 (88%)	139 (87%)	20 (13%)	4	14
1	H	161/181 (89%)	135 (84%)	26 (16%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	158/181 (87%)	131 (83%)	27 (17%)	2	6
1	J	159/181 (88%)	142 (89%)	17 (11%)	6	20
All	All	1588/1810 (88%)	1381 (87%)	207 (13%)	4	13

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	0.53	0	4,8,8	1.00	0
2	DTU	E	201	-	7,7,7	0.60	0	4,8,8	1.37	1 (25%)
2	DTU	G	201	-	7,7,7	0.64	0	4,8,8	0.74	0
3	DTV	C	201	-	7,7,7	0.72	0	4,8,8	0.52	0
2	DTU	H	201	-	7,7,7	0.83	0	4,8,8	1.59	2 (50%)
2	DTU	J	201	-	7,7,7	0.65	0	4,8,8	0.47	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	-	-	6/8/8/8	-
2	DTU	E	201	-	-	5/8/8/8	-
2	DTU	G	201	-	-	2/8/8/8	-
3	DTV	C	201	-	-	4/8/8/8	-
2	DTU	H	201	-	-	6/8/8/8	-
2	DTU	J	201	-	-	8/8/8/8	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	DTU	O2-C2-C3	2.24	114.32	109.72
2	H	201	DTU	O3-C3-C2	-2.09	105.43	109.72
2	E	201	DTU	C3-C4-S4	-2.07	108.45	114.47

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
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
2	E	201	DTU	2	0
2	G	201	DTU	3	0
3	C	201	DTV	1	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, 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%)	-0.29	0 100 100	3, 10, 25, 44	0
1	B	197/216 (91%)	-0.17	1 (0%) 91 88	3, 11, 25, 42	0
1	C	196/216 (90%)	-0.16	0 100 100	4, 12, 26, 44	0
1	D	194/216 (89%)	-0.36	0 100 100	5, 13, 24, 40	0
1	E	195/216 (90%)	-0.16	1 (0%) 91 88	4, 11, 23, 48	0
1	F	194/216 (89%)	-0.18	0 100 100	6, 13, 25, 39	0
1	G	195/216 (90%)	-0.20	0 100 100	3, 11, 25, 46	0
1	H	195/216 (90%)	-0.23	0 100 100	4, 12, 24, 44	0
1	I	195/216 (90%)	-0.20	0 100 100	4, 11, 25, 44	0
1	J	195/216 (90%)	-0.17	0 100 100	4, 12, 23, 45	0
All	All	1951/2160 (90%)	-0.21	2 (0%) 95 95	3, 12, 25, 48	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	192	ALA	2.4
1	B	0	MET	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. 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(\AA^2)	Q<0.9
2	DTU	E	201	8/8	0.81	0.28	49,57,63,70	0
2	DTU	B	201	8/8	0.83	0.23	47,51,54,58	0
2	DTU	G	201	8/8	0.85	0.22	55,58,62,66	0
3	DTV	C	201	8/8	0.85	0.23	56,59,63,67	0
2	DTU	H	201	8/8	0.87	0.25	45,53,58,64	0
2	DTU	J	201	8/8	0.87	0.27	57,59,64,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.