wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 02:58 PM EDT

PDB ID	:	6UTL
Title	:	Yeast Thiol Specific antoxidant 2 with C171S mutation and catalytic cysteine alkylated with iodoacetamide
Authors	:	Tairum, C.A.; Bannitz-Fernandes, R.; Tonoli, C.C.C.; Murakami, M.T.; de Oliveira, M.A.; Netto, L.E.S.
Deposited on	:	2019-10-29
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

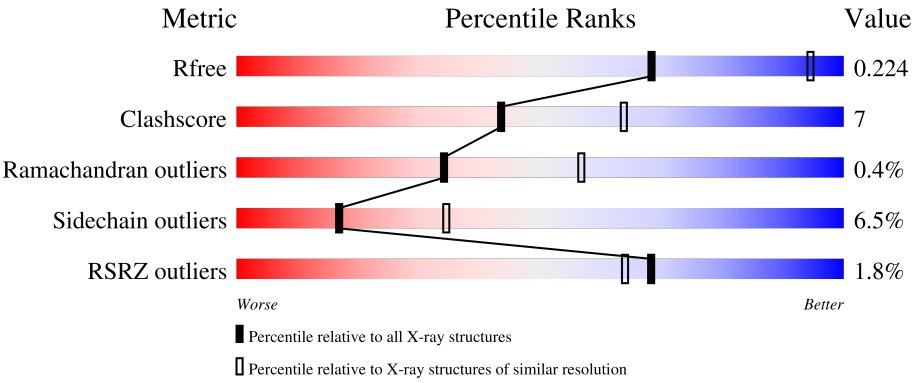
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	58% 16% 23%
1	B	216	62% 12% 24%
1	C	216	60% 12% 23%
1	D	216	62% 11% 24%
1	E	216	61% 10% 24%

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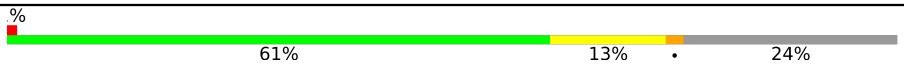
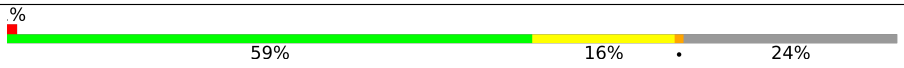
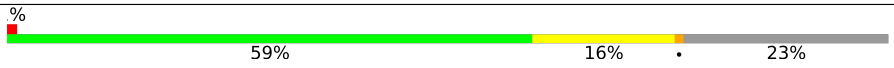
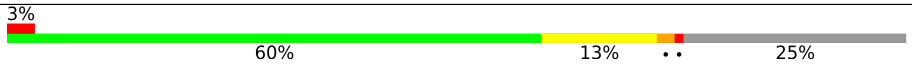
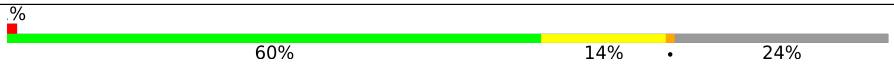
Mol	Chain	Length	Quality of chain
1	F	216	
1	G	216	
1	H	216	
1	I	216	
1	J	216	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12817 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
1	A	167	Total	C	N	O	S	0	0	0
			1286	831	213	241	1			
1	B	165	Total	C	N	O	S	0	0	0
			1266	817	212	236	1			
1	C	166	Total	C	N	O	S	0	0	0
			1284	831	214	238	1			
1	D	165	Total	C	N	O	S	0	0	0
			1282	831	213	236	2			
1	E	164	Total	C	N	O	S	0	0	0
			1275	826	213	235	1			
1	F	165	Total	C	N	O	S	0	0	0
			1271	825	212	232	2			
1	G	165	Total	C	N	O	S	0	0	0
			1278	827	212	238	1			
1	H	167	Total	C	N	O	S	0	0	0
			1302	843	217	241	1			
1	I	163	Total	C	N	O	S	0	0	0
			1270	824	210	235	1			
1	J	164	Total	C	N	O	S	0	0	0
			1279	829	213	236	1			

There are 210 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q04120
A	-18	GLY	-	expression tag	UNP Q04120
A	-17	SER	-	expression tag	UNP Q04120
A	-16	SER	-	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	HIS	-	expression tag	UNP Q04120
A	-11	HIS	-	expression tag	UNP Q04120

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	HIS	-	expression tag	UNP Q04120
A	-9	SER	-	expression tag	UNP Q04120
A	-8	SER	-	expression tag	UNP Q04120
A	-7	GLY	-	expression tag	UNP Q04120
A	-6	LEU	-	expression tag	UNP Q04120
A	-5	VAL	-	expression tag	UNP Q04120
A	-4	PRO	-	expression tag	UNP Q04120
A	-3	ARG	-	expression tag	UNP Q04120
A	-2	GLY	-	expression tag	UNP Q04120
A	-1	SER	-	expression tag	UNP Q04120
A	0	HIS	-	expression tag	UNP Q04120
A	171	SER	CYS	engineered mutation	UNP Q04120
B	-19	MET	-	initiating methionine	UNP Q04120
B	-18	GLY	-	expression tag	UNP Q04120
B	-17	SER	-	expression tag	UNP Q04120
B	-16	SER	-	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	HIS	-	expression tag	UNP Q04120
B	-11	HIS	-	expression tag	UNP Q04120
B	-10	HIS	-	expression tag	UNP Q04120
B	-9	SER	-	expression tag	UNP Q04120
B	-8	SER	-	expression tag	UNP Q04120
B	-7	GLY	-	expression tag	UNP Q04120
B	-6	LEU	-	expression tag	UNP Q04120
B	-5	VAL	-	expression tag	UNP Q04120
B	-4	PRO	-	expression tag	UNP Q04120
B	-3	ARG	-	expression tag	UNP Q04120
B	-2	GLY	-	expression tag	UNP Q04120
B	-1	SER	-	expression tag	UNP Q04120
B	0	HIS	-	expression tag	UNP Q04120
B	171	SER	CYS	engineered mutation	UNP Q04120
C	-19	MET	-	initiating methionine	UNP Q04120
C	-18	GLY	-	expression tag	UNP Q04120
C	-17	SER	-	expression tag	UNP Q04120
C	-16	SER	-	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	HIS	-	expression tag	UNP Q04120
C	-11	HIS	-	expression tag	UNP Q04120

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	expression tag	UNP Q04120
C	-9	SER	-	expression tag	UNP Q04120
C	-8	SER	-	expression tag	UNP Q04120
C	-7	GLY	-	expression tag	UNP Q04120
C	-6	LEU	-	expression tag	UNP Q04120
C	-5	VAL	-	expression tag	UNP Q04120
C	-4	PRO	-	expression tag	UNP Q04120
C	-3	ARG	-	expression tag	UNP Q04120
C	-2	GLY	-	expression tag	UNP Q04120
C	-1	SER	-	expression tag	UNP Q04120
C	0	HIS	-	expression tag	UNP Q04120
C	171	SER	CYS	engineered mutation	UNP Q04120
D	-19	MET	-	initiating methionine	UNP Q04120
D	-18	GLY	-	expression tag	UNP Q04120
D	-17	SER	-	expression tag	UNP Q04120
D	-16	SER	-	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	HIS	-	expression tag	UNP Q04120
D	-11	HIS	-	expression tag	UNP Q04120
D	-10	HIS	-	expression tag	UNP Q04120
D	-9	SER	-	expression tag	UNP Q04120
D	-8	SER	-	expression tag	UNP Q04120
D	-7	GLY	-	expression tag	UNP Q04120
D	-6	LEU	-	expression tag	UNP Q04120
D	-5	VAL	-	expression tag	UNP Q04120
D	-4	PRO	-	expression tag	UNP Q04120
D	-3	ARG	-	expression tag	UNP Q04120
D	-2	GLY	-	expression tag	UNP Q04120
D	-1	SER	-	expression tag	UNP Q04120
D	0	HIS	-	expression tag	UNP Q04120
D	171	SER	CYS	engineered mutation	UNP Q04120
E	-19	MET	-	initiating methionine	UNP Q04120
E	-18	GLY	-	expression tag	UNP Q04120
E	-17	SER	-	expression tag	UNP Q04120
E	-16	SER	-	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	HIS	-	expression tag	UNP Q04120
E	-11	HIS	-	expression tag	UNP Q04120

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP Q04120
E	-9	SER	-	expression tag	UNP Q04120
E	-8	SER	-	expression tag	UNP Q04120
E	-7	GLY	-	expression tag	UNP Q04120
E	-6	LEU	-	expression tag	UNP Q04120
E	-5	VAL	-	expression tag	UNP Q04120
E	-4	PRO	-	expression tag	UNP Q04120
E	-3	ARG	-	expression tag	UNP Q04120
E	-2	GLY	-	expression tag	UNP Q04120
E	-1	SER	-	expression tag	UNP Q04120
E	0	HIS	-	expression tag	UNP Q04120
E	171	SER	CYS	engineered mutation	UNP Q04120
F	-19	MET	-	initiating methionine	UNP Q04120
F	-18	GLY	-	expression tag	UNP Q04120
F	-17	SER	-	expression tag	UNP Q04120
F	-16	SER	-	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	HIS	-	expression tag	UNP Q04120
F	-11	HIS	-	expression tag	UNP Q04120
F	-10	HIS	-	expression tag	UNP Q04120
F	-9	SER	-	expression tag	UNP Q04120
F	-8	SER	-	expression tag	UNP Q04120
F	-7	GLY	-	expression tag	UNP Q04120
F	-6	LEU	-	expression tag	UNP Q04120
F	-5	VAL	-	expression tag	UNP Q04120
F	-4	PRO	-	expression tag	UNP Q04120
F	-3	ARG	-	expression tag	UNP Q04120
F	-2	GLY	-	expression tag	UNP Q04120
F	-1	SER	-	expression tag	UNP Q04120
F	0	HIS	-	expression tag	UNP Q04120
F	171	SER	CYS	engineered mutation	UNP Q04120
G	-19	MET	-	initiating methionine	UNP Q04120
G	-18	GLY	-	expression tag	UNP Q04120
G	-17	SER	-	expression tag	UNP Q04120
G	-16	SER	-	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	HIS	-	expression tag	UNP Q04120
G	-11	HIS	-	expression tag	UNP Q04120

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-10	HIS	-	expression tag	UNP Q04120
G	-9	SER	-	expression tag	UNP Q04120
G	-8	SER	-	expression tag	UNP Q04120
G	-7	GLY	-	expression tag	UNP Q04120
G	-6	LEU	-	expression tag	UNP Q04120
G	-5	VAL	-	expression tag	UNP Q04120
G	-4	PRO	-	expression tag	UNP Q04120
G	-3	ARG	-	expression tag	UNP Q04120
G	-2	GLY	-	expression tag	UNP Q04120
G	-1	SER	-	expression tag	UNP Q04120
G	0	HIS	-	expression tag	UNP Q04120
G	171	SER	CYS	engineered mutation	UNP Q04120
H	-19	MET	-	initiating methionine	UNP Q04120
H	-18	GLY	-	expression tag	UNP Q04120
H	-17	SER	-	expression tag	UNP Q04120
H	-16	SER	-	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	HIS	-	expression tag	UNP Q04120
H	-11	HIS	-	expression tag	UNP Q04120
H	-10	HIS	-	expression tag	UNP Q04120
H	-9	SER	-	expression tag	UNP Q04120
H	-8	SER	-	expression tag	UNP Q04120
H	-7	GLY	-	expression tag	UNP Q04120
H	-6	LEU	-	expression tag	UNP Q04120
H	-5	VAL	-	expression tag	UNP Q04120
H	-4	PRO	-	expression tag	UNP Q04120
H	-3	ARG	-	expression tag	UNP Q04120
H	-2	GLY	-	expression tag	UNP Q04120
H	-1	SER	-	expression tag	UNP Q04120
H	0	HIS	-	expression tag	UNP Q04120
H	171	SER	CYS	engineered mutation	UNP Q04120
I	-19	MET	-	initiating methionine	UNP Q04120
I	-18	GLY	-	expression tag	UNP Q04120
I	-17	SER	-	expression tag	UNP Q04120
I	-16	SER	-	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	HIS	-	expression tag	UNP Q04120
I	-11	HIS	-	expression tag	UNP Q04120

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-10	HIS	-	expression tag	UNP Q04120
I	-9	SER	-	expression tag	UNP Q04120
I	-8	SER	-	expression tag	UNP Q04120
I	-7	GLY	-	expression tag	UNP Q04120
I	-6	LEU	-	expression tag	UNP Q04120
I	-5	VAL	-	expression tag	UNP Q04120
I	-4	PRO	-	expression tag	UNP Q04120
I	-3	ARG	-	expression tag	UNP Q04120
I	-2	GLY	-	expression tag	UNP Q04120
I	-1	SER	-	expression tag	UNP Q04120
I	0	HIS	-	expression tag	UNP Q04120
I	171	SER	CYS	engineered mutation	UNP Q04120
J	-19	MET	-	initiating methionine	UNP Q04120
J	-18	GLY	-	expression tag	UNP Q04120
J	-17	SER	-	expression tag	UNP Q04120
J	-16	SER	-	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	HIS	-	expression tag	UNP Q04120
J	-11	HIS	-	expression tag	UNP Q04120
J	-10	HIS	-	expression tag	UNP Q04120
J	-9	SER	-	expression tag	UNP Q04120
J	-8	SER	-	expression tag	UNP Q04120
J	-7	GLY	-	expression tag	UNP Q04120
J	-6	LEU	-	expression tag	UNP Q04120
J	-5	VAL	-	expression tag	UNP Q04120
J	-4	PRO	-	expression tag	UNP Q04120
J	-3	ARG	-	expression tag	UNP Q04120
J	-2	GLY	-	expression tag	UNP Q04120
J	-1	SER	-	expression tag	UNP Q04120
J	0	HIS	-	expression tag	UNP Q04120
J	171	SER	CYS	engineered mutation	UNP Q04120

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total O 5 5	0	0
2	B	2	Total O 2 2	0	0
2	C	6	Total O 6 6	0	0

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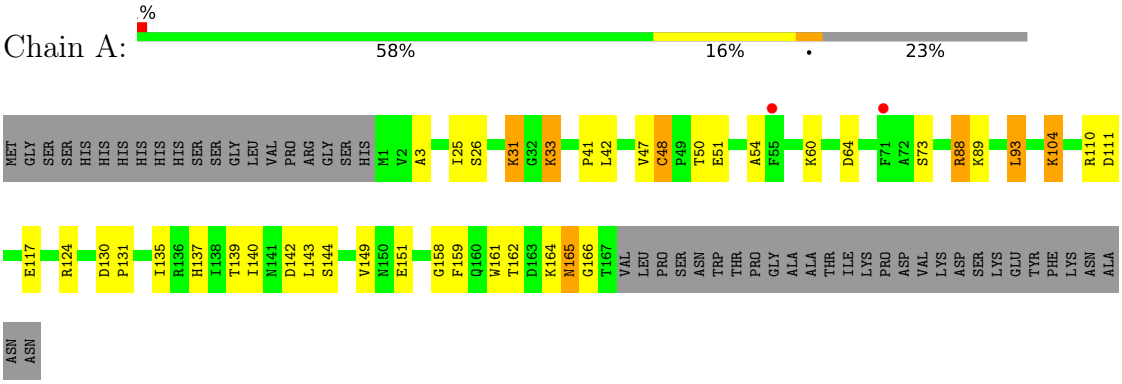
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total O 2 2	0	0
2	E	1	Total O 1 1	0	0
2	F	1	Total O 1 1	0	0
2	G	2	Total O 2 2	0	0
2	H	3	Total O 3 3	0	0
2	J	2	Total O 2 2	0	0

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.

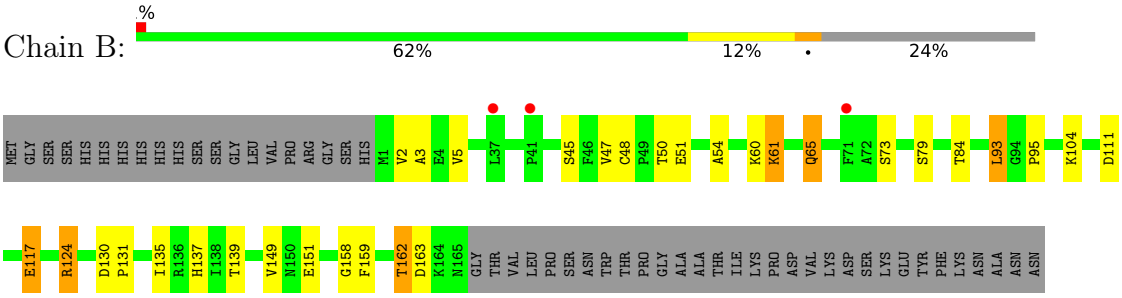
• Molecule 1: Peroxiredoxin TSA2

Chain A:



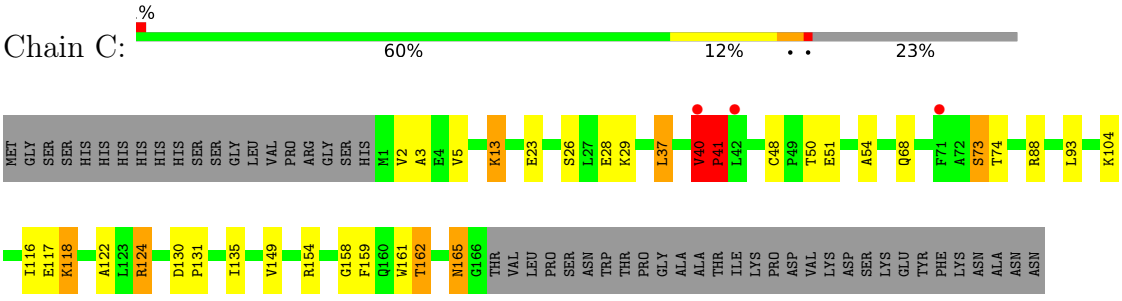
• Molecule 1: Peroxiredoxin TSA2

Chain B:



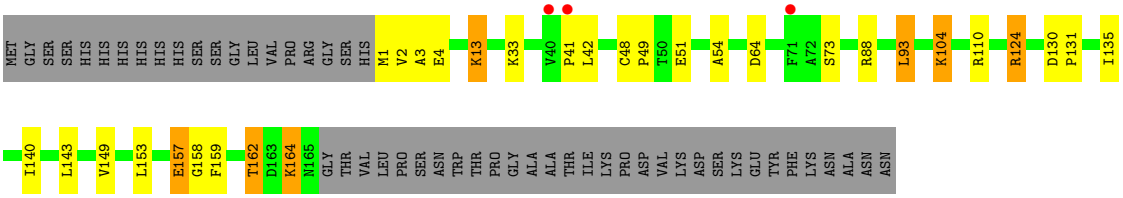
• Molecule 1: Peroxiredoxin TSA2

Chain C:



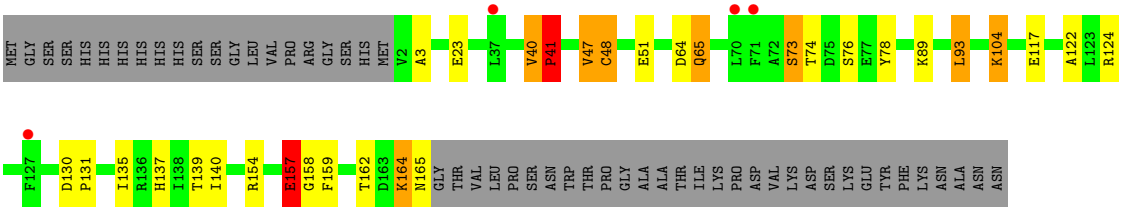
• Molecule 1: Peroxiredoxin TSA2

Chain D:



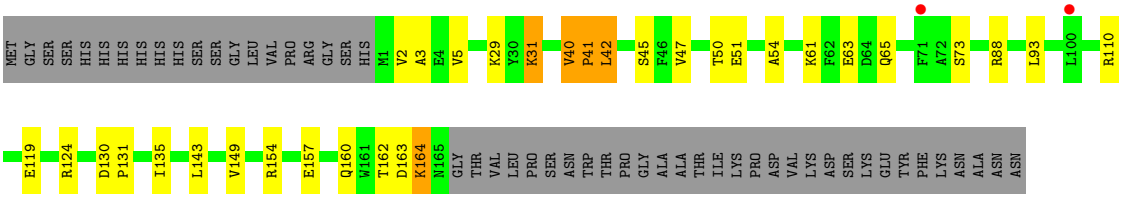
• Molecule 1: Peroxiredoxin TSA2

Chain E:



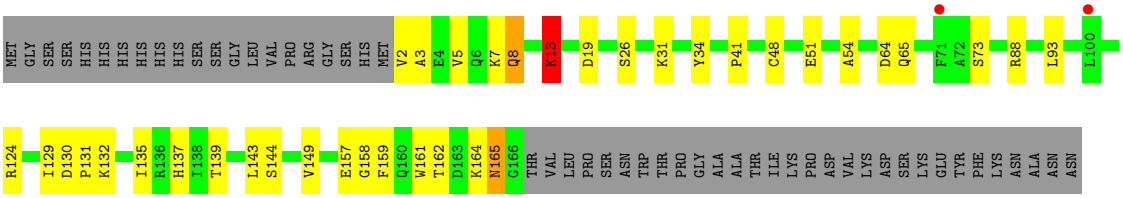
• Molecule 1: Peroxiredoxin TSA2

Chain F:



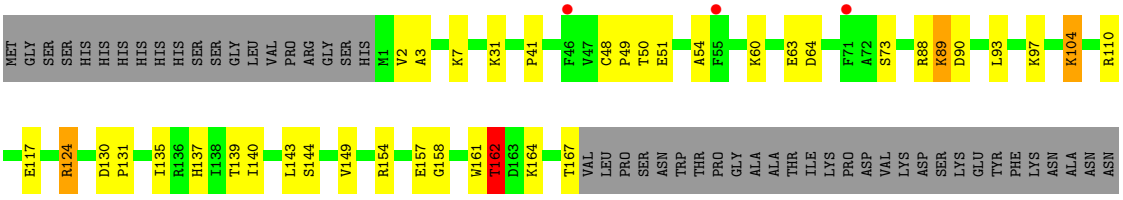
• Molecule 1: Peroxiredoxin TSA2

Chain G:



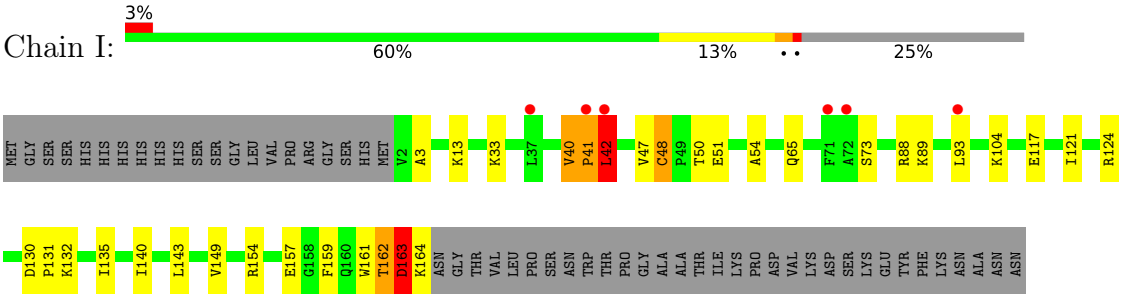
• Molecule 1: Peroxiredoxin TSA2

Chain H:



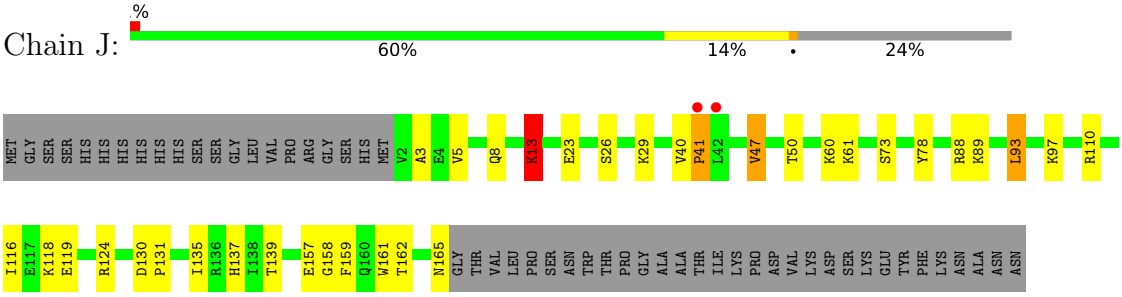
• Molecule 1: Peroxiredoxin TSA2

Chain I:



• Molecule 1: Peroxiredoxin TSA2

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.37Å 177.31Å 115.26Å 90.00° 103.28° 90.00°	Depositor
Resolution (Å)	47.40 – 2.60 47.40 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.40-2.60) 97.7 (47.40-2.61)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.198 , 0.229 0.196 , 0.224	Depositor DCC
R_{free} test set	3018 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	76.0	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.210 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.733 for H, K, L 0.267 for -H, -K, H+L	Depositor
Outliers	0 of 62339 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12817	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: YCM

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	0.94	1/1302 (0.1%)	1.08	6/1767 (0.3%)
1	B	0.99	1/1281 (0.1%)	1.02	6/1738 (0.3%)
1	C	1.01	2/1300 (0.2%)	1.13	11/1760 (0.6%)
1	D	0.97	1/1298 (0.1%)	1.06	8/1758 (0.5%)
1	E	1.03	5/1291 (0.4%)	1.12	9/1748 (0.5%)
1	F	0.99	2/1287 (0.2%)	1.14	12/1745 (0.7%)
1	G	0.91	0/1294	1.06	7/1754 (0.4%)
1	H	0.92	1/1318 (0.1%)	1.06	7/1783 (0.4%)
1	I	0.95	2/1286 (0.2%)	1.24	15/1742 (0.9%)
1	J	0.98	2/1295 (0.2%)	1.12	8/1752 (0.5%)
All	All	0.97	17/12952 (0.1%)	1.10	89/17547 (0.5%)

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	C	0	3
1	D	0	1
1	E	0	2
1	F	0	2
1	I	0	3
All	All	0	11

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	119	GLU	CG-CD	-7.01	1.41	1.51
1	A	144	SER	CB-OG	-6.79	1.33	1.42
1	C	41	PRO	C-O	6.68	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	157	GLU	CD-OE2	6.48	1.32	1.25
1	E	41	PRO	CA-C	-6.32	1.40	1.52

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	42	LEU	CA-CB-CG	15.13	150.10	115.30
1	J	110	ARG	NE-CZ-NH1	-11.07	114.77	120.30
1	A	33	LYS	CA-CB-CG	10.38	136.24	113.40
1	F	31	LYS	CD-CE-NZ	-10.09	88.49	111.70
1	I	40	VAL	N-CA-C	10.05	138.15	111.00

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	40	VAL	Peptide
1	C	41	PRO	Mainchain,Peptide
1	D	164	LYS	Mainchain
1	E	41	PRO	Mainchain,Peptide
1	F	41	PRO	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	1286	0	1281	27	0
1	B	1266	0	1262	16	0
1	C	1284	0	1292	21	0
1	D	1282	0	1296	15	0
1	E	1275	0	1286	20	4
1	F	1271	0	1279	13	0
1	G	1278	0	1280	23	0
1	H	1302	0	1325	18	0
1	I	1270	0	1281	11	4
1	J	1279	0	1295	18	0
2	A	5	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	6	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	1	0
2	G	2	0	0	7	0
2	H	3	0	0	1	0
2	J	2	0	0	0	0
All	All	12817	0	12877	172	4

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 7.

The worst 5 of 172 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:A:25:ILE:HG22	2:A:201:HOH:O	1.46	1.12
1:A:142:ASP:HB3	2:A:203:HOH:O	1.57	1.04
1:E:65:GLN:HG3	1:E:157:GLU:OE1	1.61	0.98
1:H:89:LYS:NZ	1:H:90:ASP:OD2	2.02	0.93
1:A:165:ASN:N	1:A:165:ASN:HD22	1.70	0.89

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:YCM:OZ1	1:I:161:TRP:CG[1_556]	1.93	0.27
1:E:48:YCM:OZ1	1:I:161:TRP:CD2[1_556]	1.95	0.25
1:E:48:YCM:NZ2	1:I:161:TRP:CZ2[1_556]	2.07	0.13
1:E:48:YCM:NZ2	1:I:161:TRP:CE2[1_556]	2.18	0.02

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	164/216 (76%)	151 (92%)	12 (7%)	1 (1%)	25 47
1	B	162/216 (75%)	152 (94%)	10 (6%)	0	100 100
1	C	163/216 (76%)	151 (93%)	11 (7%)	1 (1%)	25 47
1	D	162/216 (75%)	151 (93%)	11 (7%)	0	100 100
1	E	161/216 (74%)	151 (94%)	9 (6%)	1 (1%)	25 47
1	F	162/216 (75%)	150 (93%)	11 (7%)	1 (1%)	25 47
1	G	162/216 (75%)	152 (94%)	10 (6%)	0	100 100
1	H	164/216 (76%)	152 (93%)	11 (7%)	1 (1%)	25 47
1	I	160/216 (74%)	148 (92%)	11 (7%)	1 (1%)	25 47
1	J	161/216 (74%)	151 (94%)	10 (6%)	0	100 100
All	All	1621/2160 (75%)	1509 (93%)	106 (6%)	6 (0%)	34 57

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	42	LEU
1	I	163	ASP
1	C	40	VAL
1	E	40	VAL
1	H	49	PRO

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	134/181 (74%)	123 (92%)	11 (8%)	11 22
1	B	131/181 (72%)	122 (93%)	9 (7%)	15 31
1	C	134/181 (74%)	125 (93%)	9 (7%)	16 33
1	D	135/181 (75%)	128 (95%)	7 (5%)	23 46
1	E	134/181 (74%)	126 (94%)	8 (6%)	19 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	132/181 (73%)	129 (98%)	3 (2%)	50 75
1	G	134/181 (74%)	126 (94%)	8 (6%)	19 39
1	H	138/181 (76%)	127 (92%)	11 (8%)	12 24
1	I	134/181 (74%)	126 (94%)	8 (6%)	19 39
1	J	135/181 (75%)	122 (90%)	13 (10%)	8 16
All	All	1341/1810 (74%)	1254 (94%)	87 (6%)	17 34

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	50	THR
1	I	117	GLU
1	H	89	LYS
1	H	164	LYS
1	J	41	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	8	GLN
1	J	8	GLN
1	I	65	GLN
1	E	8	GLN
1	G	165	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)

10 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	YCM	C	48	1	7,9,10	0.58	0	4,10,12	1.54	1 (25%)
1	YCM	B	48	1	7,9,10	1.50	0	4,10,12	2.02	2 (50%)
1	YCM	F	48	1	7,9,10	0.95	0	4,10,12	1.29	0
1	YCM	G	48	1	7,9,10	1.22	1 (14%)	4,10,12	1.70	2 (50%)
1	YCM	D	48	1	7,9,10	0.70	0	4,10,12	1.48	0
1	YCM	E	48	1	7,9,10	1.37	1 (14%)	4,10,12	3.81	2 (50%)
1	YCM	H	48	1	7,9,10	1.10	1 (14%)	4,10,12	2.27	1 (25%)
1	YCM	J	48	1	7,9,10	0.96	0	4,10,12	1.17	0
1	YCM	A	48	1	7,9,10	2.24	2 (28%)	4,10,12	3.60	1 (25%)
1	YCM	I	48	1	7,9,10	1.52	1 (14%)	4,10,12	2.67	1 (25%)

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
1	YCM	C	48	1	-	3/6/8/10	-
1	YCM	B	48	1	-	2/6/8/10	-
1	YCM	F	48	1	-	3/6/8/10	-
1	YCM	G	48	1	-	3/6/8/10	-
1	YCM	D	48	1	-	5/6/8/10	-
1	YCM	E	48	1	-	4/6/8/10	-
1	YCM	H	48	1	-	2/6/8/10	-
1	YCM	J	48	1	-	3/6/8/10	-
1	YCM	A	48	1	-	3/6/8/10	-
1	YCM	I	48	1	-	3/6/8/10	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	YCM	CB-SG	-4.36	1.63	1.80
1	I	48	YCM	CB-CA	-3.39	1.45	1.53
1	A	48	YCM	CB-CA	-3.21	1.45	1.53
1	E	48	YCM	CD-SG	-3.13	1.73	1.81
1	G	48	YCM	CB-SG	-2.45	1.71	1.80

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	48	YCM	CE-CD-SG	-7.18	92.46	113.59
1	E	48	YCM	CE-CD-SG	-6.87	93.37	113.59
1	I	48	YCM	CA-CB-SG	-5.09	95.11	113.74
1	H	48	YCM	CE-CD-SG	-3.29	103.90	113.59
1	B	48	YCM	CE-CD-SG	-3.14	104.33	113.59

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	48	YCM	CE-CD-SG-CB
1	A	48	YCM	SG-CD-CE-OZ1
1	A	48	YCM	SG-CD-CE-NZ2
1	B	48	YCM	CE-CD-SG-CB
1	B	48	YCM	SG-CD-CE-NZ2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	48	YCM	1	0
1	E	48	YCM	0	4
1	A	48	YCM	2	0
1	I	48	YCM	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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

6.1 Protein, DNA and RNA chains

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^{th} 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	166/216 (76%)	0.01	2 (1%)	79	76	59, 75, 97, 114	0
1	B	164/216 (75%)	-0.08	3 (1%)	68	64	59, 73, 87, 109	0
1	C	165/216 (76%)	-0.10	3 (1%)	68	64	58, 73, 90, 100	0
1	D	164/216 (75%)	-0.04	3 (1%)	68	64	57, 69, 82, 94	0
1	E	163/216 (75%)	-0.08	4 (2%)	57	51	57, 70, 85, 99	0
1	F	164/216 (75%)	-0.10	2 (1%)	79	76	61, 76, 95, 109	0
1	G	164/216 (75%)	-0.14	2 (1%)	79	76	63, 75, 85, 92	0
1	H	166/216 (76%)	0.00	3 (1%)	68	64	62, 74, 90, 102	0
1	I	162/216 (75%)	0.01	6 (3%)	41	34	64, 79, 96, 103	0
1	J	163/216 (75%)	-0.09	2 (1%)	79	76	59, 77, 97, 118	0
All	All	1641/2160 (75%)	-0.06	30 (1%)	68	64	57, 74, 92, 118	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	41	PRO	3.8
1	B	71	PHE	3.4
1	A	71	PHE	3.4
1	H	46	PHE	3.3
1	I	41	PRO	3.2

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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
1	YCM	B	48	10/11	0.79	0.15	91,99,103,107	0
1	YCM	H	48	10/11	0.81	0.21	76,90,95,99	0
1	YCM	J	48	10/11	0.84	0.22	89,98,103,105	0
1	YCM	G	48	10/11	0.86	0.16	81,88,91,92	0
1	YCM	I	48	10/11	0.87	0.17	78,103,110,111	0
1	YCM	C	48	10/11	0.87	0.15	72,97,101,105	0
1	YCM	A	48	10/11	0.89	0.14	79,87,100,104	0
1	YCM	D	48	10/11	0.92	0.10	79,86,90,97	0
1	YCM	F	48	10/11	0.93	0.08	87,94,109,110	0
1	YCM	E	48	10/11	0.95	0.09	79,88,112,120	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.