



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:22 pm GMT

PDB ID : 3TKQ
Title : Crystal structure of full-length human peroxiredoxin 4 with mixed conformation
Authors : Wang, X.; Wang, L.; Wang, X.; Sun, F.; Wang, C.-C.
Deposited on : 2011-08-28
Resolution : 2.22 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

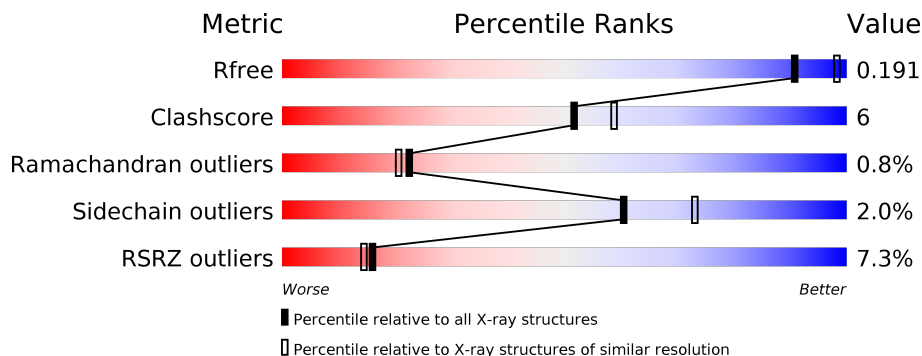
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	100719	4744 (2.24-2.20)
Clashscore	112137	5509 (2.24-2.20)
Ramachandran outliers	110173	5427 (2.24-2.20)
Sidechain outliers	110143	5428 (2.24-2.20)
RSRZ outliers	101464	4776 (2.24-2.20)

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. 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	246	<div> <div>13%</div> <div> <div></div> <div>65%</div> <div>11%</div> <div>22%</div> </div> </div>
1	B	246	<div> <div>8%</div> <div> <div></div> <div>65%</div> <div>9%</div> <div>25%</div> </div> </div>
1	C	246	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>8%</div> <div>33%</div> </div> </div>
1	D	246	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>6%</div> <div>33%</div> </div> </div>
1	E	246	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>10%</div> <div>33%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7604 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-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	8	0
			1584	1030	259	291	4			
1	B	185	Total	C	N	O	S	0	8	0
			1540	999	253	284	4			
1	C	166	Total	C	N	O	S	0	8	0
			1407	913	232	259	3			
1	D	165	Total	C	N	O	S	0	1	0
			1339	866	223	248	2			
1	E	166	Total	C	N	O	S	0	7	0
			1398	908	231	256	3			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q13162
A	-10	ARG	-	EXPRESSION TAG	UNP Q13162
A	-9	GLY	-	EXPRESSION TAG	UNP Q13162
A	-8	SER	-	EXPRESSION TAG	UNP Q13162
A	-7	HIS	-	EXPRESSION TAG	UNP Q13162
A	-6	HIS	-	EXPRESSION TAG	UNP Q13162
A	-5	HIS	-	EXPRESSION TAG	UNP Q13162
A	-4	HIS	-	EXPRESSION TAG	UNP Q13162
A	-3	HIS	-	EXPRESSION TAG	UNP Q13162
A	-2	HIS	-	EXPRESSION TAG	UNP Q13162
A	-1	GLY	-	EXPRESSION TAG	UNP Q13162
A	0	SER	-	EXPRESSION TAG	UNP Q13162
B	-11	MET	-	EXPRESSION TAG	UNP Q13162
B	-10	ARG	-	EXPRESSION TAG	UNP Q13162
B	-9	GLY	-	EXPRESSION TAG	UNP Q13162
B	-8	SER	-	EXPRESSION TAG	UNP Q13162
B	-7	HIS	-	EXPRESSION TAG	UNP Q13162
B	-6	HIS	-	EXPRESSION TAG	UNP Q13162
B	-5	HIS	-	EXPRESSION TAG	UNP Q13162

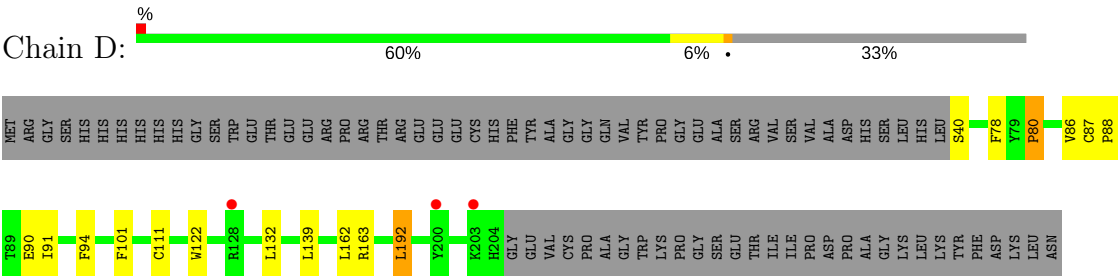
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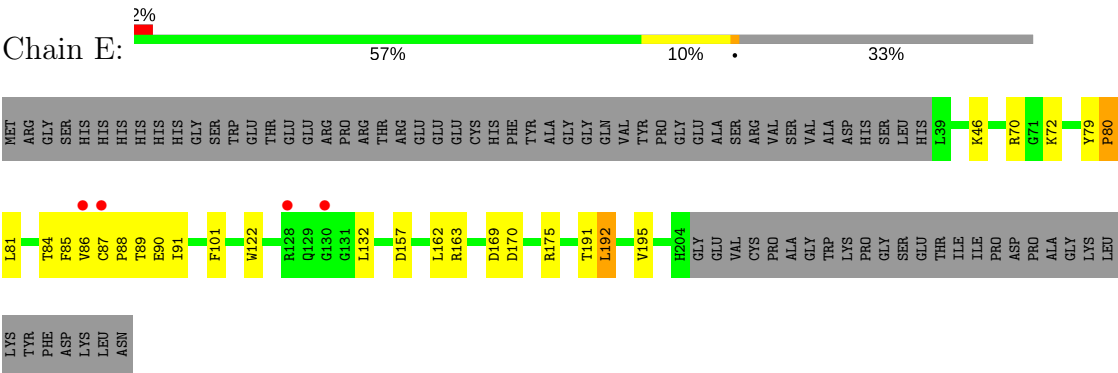
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	EXPRESSION TAG	UNP Q13162
B	-3	HIS	-	EXPRESSION TAG	UNP Q13162
B	-2	HIS	-	EXPRESSION TAG	UNP Q13162
B	-1	GLY	-	EXPRESSION TAG	UNP Q13162
B	0	SER	-	EXPRESSION TAG	UNP Q13162
C	-11	MET	-	EXPRESSION TAG	UNP Q13162
C	-10	ARG	-	EXPRESSION TAG	UNP Q13162
C	-9	GLY	-	EXPRESSION TAG	UNP Q13162
C	-8	SER	-	EXPRESSION TAG	UNP Q13162
C	-7	HIS	-	EXPRESSION TAG	UNP Q13162
C	-6	HIS	-	EXPRESSION TAG	UNP Q13162
C	-5	HIS	-	EXPRESSION TAG	UNP Q13162
C	-4	HIS	-	EXPRESSION TAG	UNP Q13162
C	-3	HIS	-	EXPRESSION TAG	UNP Q13162
C	-2	HIS	-	EXPRESSION TAG	UNP Q13162
C	-1	GLY	-	EXPRESSION TAG	UNP Q13162
C	0	SER	-	EXPRESSION TAG	UNP Q13162
D	-11	MET	-	EXPRESSION TAG	UNP Q13162
D	-10	ARG	-	EXPRESSION TAG	UNP Q13162
D	-9	GLY	-	EXPRESSION TAG	UNP Q13162
D	-8	SER	-	EXPRESSION TAG	UNP Q13162
D	-7	HIS	-	EXPRESSION TAG	UNP Q13162
D	-6	HIS	-	EXPRESSION TAG	UNP Q13162
D	-5	HIS	-	EXPRESSION TAG	UNP Q13162
D	-4	HIS	-	EXPRESSION TAG	UNP Q13162
D	-3	HIS	-	EXPRESSION TAG	UNP Q13162
D	-2	HIS	-	EXPRESSION TAG	UNP Q13162
D	-1	GLY	-	EXPRESSION TAG	UNP Q13162
D	0	SER	-	EXPRESSION TAG	UNP Q13162
E	-11	MET	-	EXPRESSION TAG	UNP Q13162
E	-10	ARG	-	EXPRESSION TAG	UNP Q13162
E	-9	GLY	-	EXPRESSION TAG	UNP Q13162
E	-8	SER	-	EXPRESSION TAG	UNP Q13162
E	-7	HIS	-	EXPRESSION TAG	UNP Q13162
E	-6	HIS	-	EXPRESSION TAG	UNP Q13162
E	-5	HIS	-	EXPRESSION TAG	UNP Q13162
E	-4	HIS	-	EXPRESSION TAG	UNP Q13162
E	-3	HIS	-	EXPRESSION TAG	UNP Q13162
E	-2	HIS	-	EXPRESSION TAG	UNP Q13162
E	-1	GLY	-	EXPRESSION TAG	UNP Q13162
E	0	SER	-	EXPRESSION TAG	UNP Q13162

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	47	Total 47	O 47	0	0
2	B	77	Total 77	O 77	0	0
2	C	70	Total 70	O 70	0	0
2	D	74	Total 74	O 74	0	0
2	E	68	Total 68	O 68	0	0



● Molecule 1: Peroxiredoxin-4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.49Å 139.52Å 96.20Å 90.00° 103.38° 90.00°	Depositor
Resolution (Å)	38.86 – 2.22 38.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (38.86-2.22) 98.2 (38.86-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.186 , 0.224 0.184 , 0.191	Depositor DCC
R_{free} test set	3435 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7604	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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	0.33	0/1631	0.50	0/2217
1	B	0.40	0/1585	0.55	0/2156
1	C	0.40	0/1443	0.56	0/1959
1	D	0.42	0/1375	0.57	0/1865
1	E	0.38	0/1434	0.55	0/1947
All	All	0.39	0/7468	0.55	0/10144

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1584	0	1565	22	0
1	B	1540	0	1525	20	0
1	C	1407	0	1394	18	0
1	D	1339	0	1329	12	0
1	E	1398	0	1388	21	0
2	A	47	0	0	0	0
2	B	77	0	0	1	0
2	C	70	0	0	1	0
2	D	74	0	0	1	0
2	E	68	0	0	1	0
All	All	7604	0	7201	93	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 6.

The worst 5 of 93 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:D:80:PRO:HD2	1:D:87:CYS:SG	2.06	0.96
1:A:88[B]:PRO:HG3	1:A:122:TRP:HZ2	1.33	0.94
1:B:88[B]:PRO:HG3	1:B:122:TRP:HZ2	1.30	0.94
1:B:70:ARG:HD3	2:B:276:HOH:O	1.68	0.94
1:D:88:PRO:HG3	1:D:122:TRP:HZ2	1.36	0.90

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	197/246 (80%)	181 (92%)	13 (7%)	3 (2%)	12	8
1	B	191/246 (78%)	174 (91%)	15 (8%)	2 (1%)	18	15
1	C	172/246 (70%)	162 (94%)	9 (5%)	1 (1%)	28	28
1	D	164/246 (67%)	157 (96%)	6 (4%)	1 (1%)	28	28
1	E	171/246 (70%)	159 (93%)	11 (6%)	1 (1%)	28	28
All	All	895/1230 (73%)	833 (93%)	54 (6%)	8 (1%)	22	17

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89[A]	THR
1	A	89[B]	THR
1	B	80	PRO
1	C	80	PRO
1	B	206	GLU

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	173/213 (81%)	170 (98%)	3 (2%)	66	78
1	B	170/213 (80%)	165 (97%)	5 (3%)	48	59
1	C	155/213 (73%)	152 (98%)	3 (2%)	62	75
1	D	147/213 (69%)	145 (99%)	2 (1%)	71	83
1	E	154/213 (72%)	151 (98%)	3 (2%)	62	75
All	All	799/1065 (75%)	783 (98%)	16 (2%)	60	73

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	192	LEU
1	C	39	LEU
1	D	192	LEU
1	B	162	LEU
1	E	157	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	204	HIS
1	C	204	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

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	191/246 (77%)	0.47	32 (16%) 2 2	36, 49, 81, 96	0
1	B	185/246 (75%)	0.32	20 (10%) 6 5	28, 39, 79, 101	0
1	C	166/246 (67%)	-0.04	5 (3%) 51 48	29, 40, 59, 94	0
1	D	165/246 (67%)	-0.19	3 (1%) 69 66	31, 41, 59, 94	0
1	E	166/246 (67%)	-0.07	4 (2%) 59 57	31, 40, 62, 101	0
All	All	873/1230 (70%)	0.11	64 (7%) 16 14	28, 42, 75, 101	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	PRO	10.4
1	E	87[A]	CYS	7.5
1	B	222	ASP	7.2
1	A	87[A]	CYS	6.1
1	B	87[A]	CYS	5.7

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.