



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:38 PM GMT

PDB ID : 4TXV
Title : Crystal structure of the mixed disulfide intermediate between thioredoxin-like TlpAs(C110S) and subunit II of cytochrome c oxidase CoxBPD (C233S)
Authors : Quade, N.; Abicht, H.K.; Hennecke, H.; Glockshuber, R.
Deposited on : 2014-07-07
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
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

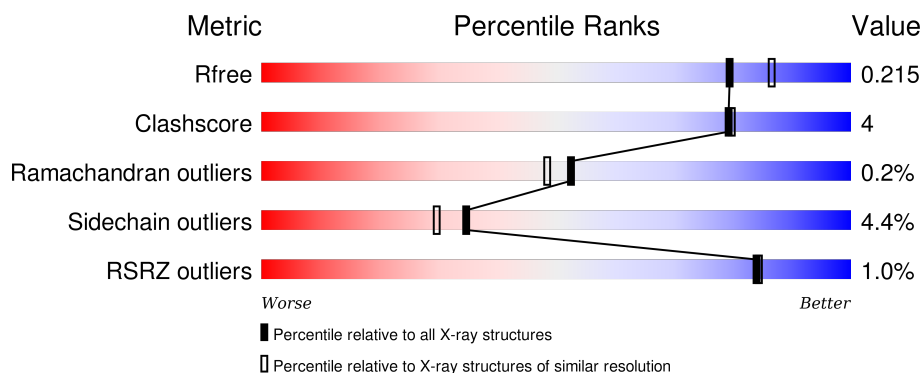
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	184	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>10% • 5%</div> </div> </div>
1	C	184	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>9% • •</div> </div> </div>
2	B	159	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>10% • • 11%</div> </div> </div>
2	D	159	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>13% 16%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5267 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 Thiol:disulfide interchange protein TlpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1314	836	226	246	6			
1	C	178	Total	C	N	O	S	0	0	0
			1335	849	230	250	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ALA	-	expression tag	UNP P43221
A	39	PRO	-	expression tag	UNP P43221
A	110	SER	CYS	engineered mutation	UNP P43221
A	218	ALA	-	expression tag	UNP P43221
A	219	ALA	-	expression tag	UNP P43221
A	220	ALA	-	expression tag	UNP P43221
A	221	LEU	-	expression tag	UNP P43221
C	38	ALA	-	expression tag	UNP P43221
C	39	PRO	-	expression tag	UNP P43221
C	110	SER	CYS	engineered mutation	UNP P43221
C	218	ALA	-	expression tag	UNP P43221
C	219	ALA	-	expression tag	UNP P43221
C	220	ALA	-	expression tag	UNP P43221
C	221	LEU	-	expression tag	UNP P43221

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total	C	N	O	S	0	0	0
			1127	735	185	202	5			
2	D	133	Total	C	N	O	S	0	0	0
			1047	684	170	188	5			

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	121	GLY	-	expression tag	UNP H7C6E5
B	122	ALA	-	expression tag	UNP H7C6E5
B	233	SER	CYS	engineered mutation	UNP H7C6E5
B	265	SER	-	expression tag	UNP H7C6E5
B	266	GLY	-	expression tag	UNP H7C6E5
B	267	GLY	-	expression tag	UNP H7C6E5
B	268	THR	-	expression tag	UNP H7C6E5
B	269	GLY	-	expression tag	UNP H7C6E5
B	270	THR	-	expression tag	UNP H7C6E5
B	271	TYR	-	expression tag	UNP H7C6E5
B	272	ALA	-	expression tag	UNP H7C6E5
B	273	SER	-	expression tag	UNP H7C6E5
B	274	ALA	-	expression tag	UNP H7C6E5
B	275	ALA	-	expression tag	UNP H7C6E5
B	276	GLY	-	expression tag	UNP H7C6E5
B	277	PRO	-	expression tag	UNP H7C6E5
B	278	THR	-	expression tag	UNP H7C6E5
B	279	GLN	-	expression tag	UNP H7C6E5
D	121	GLY	-	expression tag	UNP H7C6E5
D	122	ALA	-	expression tag	UNP H7C6E5
D	233	SER	CYS	engineered mutation	UNP H7C6E5
D	266	GLY	-	expression tag	UNP H7C6E5
D	267	GLY	-	expression tag	UNP H7C6E5
D	268	THR	-	expression tag	UNP H7C6E5
D	269	GLY	-	expression tag	UNP H7C6E5
D	270	THR	-	expression tag	UNP H7C6E5
D	271	TYR	-	expression tag	UNP H7C6E5
D	272	ALA	-	expression tag	UNP H7C6E5
D	273	SER	-	expression tag	UNP H7C6E5
D	274	ALA	-	expression tag	UNP H7C6E5
D	275	ALA	-	expression tag	UNP H7C6E5
D	276	GLY	-	expression tag	UNP H7C6E5
D	277	PRO	-	expression tag	UNP H7C6E5
D	278	THR	-	expression tag	UNP H7C6E5
D	279	GLN	-	expression tag	UNP H7C6E5

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	109	Total O 109 109	0	0
3	B	116	Total O 116 116	0	0

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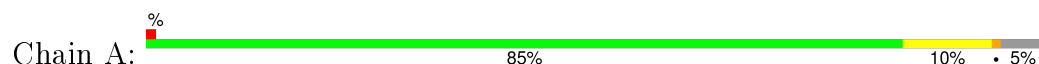
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	114	Total 114	O 114	0	0
3	D	105	Total 105	O 105	0	0

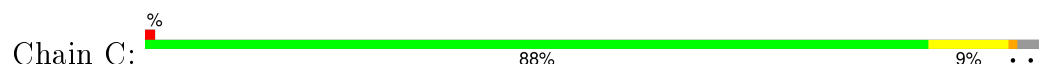
3 Residue-property plots [i](#)

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.

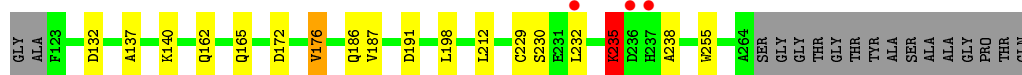
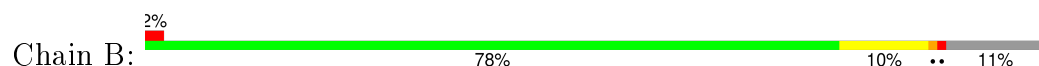
- Molecule 1: Thiol:disulfide interchange protein TlpA



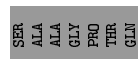
- Molecule 1: Thiol:disulfide interchange protein TlpA



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.83Å 81.64Å 109.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.42 – 2.00 49.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (65.42-2.00) 99.1 (49.25-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.163 , 0.212 0.172 , 0.215	Depositor DCC
R_{free} test set	2302 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 45681 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5267	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.82	0/1340	0.90	0/1819
1	C	0.83	0/1361	0.90	0/1847
2	B	0.87	0/1157	0.92	2/1566 (0.1%)
2	D	0.90	0/1074	0.91	1/1453 (0.1%)
All	All	0.85	0/4932	0.91	3/6685 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	172	ASP	CB-CG-OD1	5.57	123.32	118.30
2	B	132	ASP	CB-CG-OD2	5.40	123.16	118.30
2	D	172	ASP	CB-CG-OD1	5.27	123.04	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	THR	Peptide
2	B	235	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	1314	0	1343	6	0
1	C	1335	0	1368	12	0
2	B	1127	0	1122	7	0
2	D	1047	0	1042	11	0
3	A	109	0	0	0	0
3	B	116	0	0	1	0
3	C	114	0	0	1	0
3	D	105	0	0	1	0
All	All	5267	0	4875	33	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 4.

All (33) 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:C:107:CYS:HG	2:D:229:CYS:HG	1.20	0.86
1:A:107:CYS:HG	2:B:229:CYS:HG	1.27	0.83
1:C:121:GLN:O	1:C:125:SER:HB2	1.87	0.74
2:D:180:ASN:OD1	3:D:397:HOH:O	2.09	0.70
2:B:235:LYS:O	2:B:238:ALA:HB3	2.00	0.60
1:C:121:GLN:O	1:C:125:SER:CB	2.49	0.60
2:B:186:GLN:HB3	2:B:212:LEU:HD22	1.84	0.58
2:D:187:VAL:CG1	2:D:207:ALA:HB2	2.35	0.56
2:B:176:VAL:HG13	2:B:255:TRP:CZ2	2.41	0.55
2:B:230:SER:OG	2:B:232:LEU:HG	2.07	0.54
1:C:74:LYS:HE3	1:C:188:GLN:O	2.08	0.54
2:D:187:VAL:HG12	2:D:207:ALA:HB2	1.93	0.50
1:A:81:GLU:OE2	1:A:85:GLY:HA2	2.12	0.49
1:C:74:LYS:HE2	3:C:351:HOH:O	2.13	0.48
1:C:143:LYS:N	1:C:144:PRO:CD	2.77	0.47
1:A:140:ASP:O	1:A:142:GLU:N	2.48	0.47
1:A:138:THR:HG22	1:A:162:GLN:O	2.16	0.46
2:B:137:ALA:HB3	2:B:187:VAL:HG12	1.99	0.45
2:D:176:VAL:HG13	2:D:255:TRP:CZ2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:THR:HG22	1:C:216:LYS:HB2	1.99	0.44
2:D:140:LYS:O	2:D:142:TRP:HA	2.18	0.43
1:C:56:ALA:N	1:C:57:PRO:CD	2.81	0.43
2:B:176:VAL:HG13	2:B:255:TRP:CE2	2.54	0.43
1:C:97:THR:O	1:C:129:PHE:HA	2.18	0.43
2:D:147:ALA:HB2	2:D:155:GLU:HG2	2.02	0.42
1:A:97:THR:O	1:A:129:PHE:HA	2.20	0.42
1:C:74:LYS:HD2	1:C:74:LYS:HA	1.83	0.42
2:D:186:GLN:HB3	2:D:212:LEU:HD11	2.02	0.41
1:A:110:SER:HB2	1:A:180:PRO:HB3	2.02	0.41
1:C:209:LEU:HG	1:C:209:LEU:O	2.19	0.41
2:D:260:LYS:O	2:D:264:ALA:HB2	2.19	0.41
1:C:109:PRO:HD2	2:D:229:CYS:SG	2.61	0.40
3:B:407:HOH:O	2:D:128:VAL:CG1	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	173/184 (94%)	166 (96%)	6 (4%)	1 (1%)	30	22
1	C	176/184 (96%)	170 (97%)	6 (3%)	0	100	100
2	B	140/159 (88%)	135 (96%)	5 (4%)	0	100	100
2	D	129/159 (81%)	127 (98%)	2 (2%)	0	100	100
All	All	618/686 (90%)	598 (97%)	19 (3%)	1 (0%)	52	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	PRO

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	136/140 (97%)	129 (95%)	7 (5%)	29	23
1	C	138/140 (99%)	135 (98%)	3 (2%)	60	62
2	B	117/125 (94%)	110 (94%)	7 (6%)	24	17
2	D	109/125 (87%)	104 (95%)	5 (5%)	33	28
All	All	500/530 (94%)	478 (96%)	22 (4%)	35	30

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	74	LYS
1	A	94	ARG
1	A	110	SER
1	A	137	ASP
1	A	149	LYS
1	A	186	ASP
2	B	140	LYS
2	B	162	GLN
2	B	165	GLN
2	B	176	VAL
2	B	191	ASP
2	B	198	LEU
2	B	235	LYS
1	C	186	ASP
1	C	204	GLU
1	C	209	LEU
2	D	126	LEU
2	D	133	LEU
2	D	168	LEU
2	D	198	LEU
2	D	254	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	168	GLN
2	B	162	GLN
2	D	186	GLN
2	D	194	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	175/184 (95%)	-0.18	1 (0%) 90 90	22, 34, 61, 90	0
1	C	178/184 (96%)	-0.39	1 (0%) 90 90	25, 38, 58, 81	0
2	B	142/159 (89%)	-0.20	3 (2%) 67 67	23, 34, 70, 93	0
2	D	133/159 (83%)	-0.30	1 (0%) 87 88	26, 35, 65, 79	0
All	All	628/686 (91%)	-0.27	6 (0%) 84 84	22, 35, 64, 93	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	232	LEU	3.6
2	B	236	ASP	3.3
1	A	41	GLY	2.8
2	D	126	LEU	2.7
2	B	237	HIS	2.5
1	C	40	THR	2.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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.