



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:44 pm BST

PDB ID : 3UEM  
Title : Crystal structure of human PDI bb'a' domains  
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Deposited on : 2011-10-30  
Resolution : 2.29 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (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

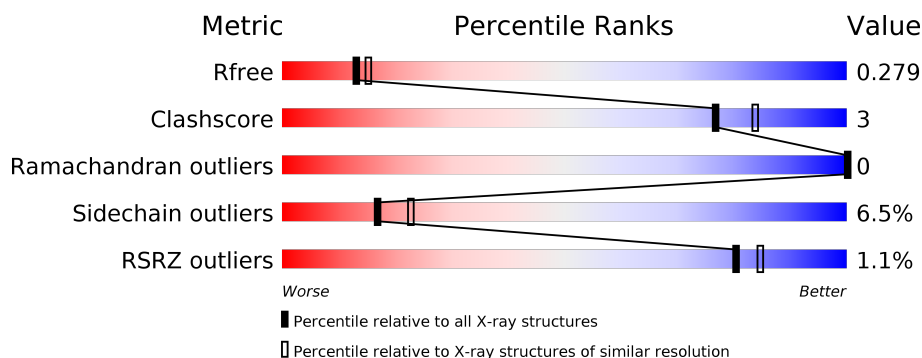
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	361	<div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3015 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.

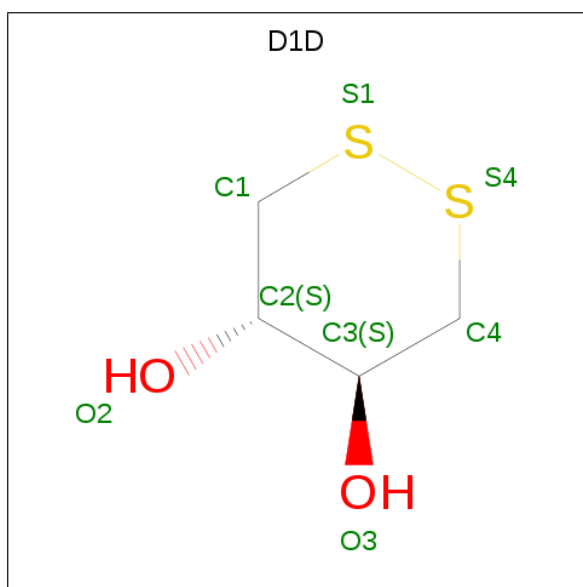
- Molecule 1 is a protein called Protein disulfide-isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	3	0
			2863	1846	462	548	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	HIS	-	EXPRESSION TAG	UNP P07237
A	120	HIS	-	EXPRESSION TAG	UNP P07237
A	121	HIS	-	EXPRESSION TAG	UNP P07237
A	122	SER	-	EXPRESSION TAG	UNP P07237
A	123	SER	-	EXPRESSION TAG	UNP P07237
A	124	GLY	-	EXPRESSION TAG	UNP P07237
A	125	LEU	-	EXPRESSION TAG	UNP P07237
A	126	GLU	-	EXPRESSION TAG	UNP P07237
A	127	VAL	-	EXPRESSION TAG	UNP P07237
A	128	LEU	-	EXPRESSION TAG	UNP P07237
A	129	PHE	-	EXPRESSION TAG	UNP P07237
A	130	GLN	-	EXPRESSION TAG	UNP P07237
A	131	GLY	-	EXPRESSION TAG	UNP P07237
A	132	PRO	-	EXPRESSION TAG	UNP P07237
A	133	GLY	-	EXPRESSION TAG	UNP P07237
A	134	SER	-	EXPRESSION TAG	UNP P07237
A	135	GLU	-	EXPRESSION TAG	UNP P07237
A	136	PHE	-	EXPRESSION TAG	UNP P07237

- Molecule 2 is (4S,5S)-1,2-DITHIANE-4,5-DIOL (three-letter code: D1D) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>S<sub>2</sub>).



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

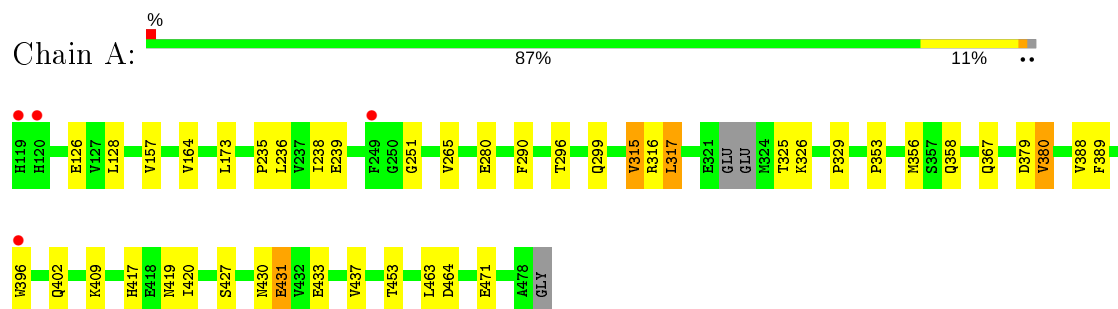
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	144	Total	O	0	0
			144	144		

### 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 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 ( $\text{RSRZ} > 2$ ). 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: Protein disulfide-isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.59Å 76.08Å 79.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.29 49.69 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.29) 99.2 (49.69-2.29)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.35 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.223 , 0.280 0.218 , 0.279	Depositor DCC
$R_{free}$ test set	906 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 35.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D1D

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	0.38	0/2942	0.53	1/3972 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	317	LEU	CA-CB-CG	7.81	133.26	115.30

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	2863	0	2780	17	0
2	A	8	0	8	0	0
3	A	144	0	0	1	0
All	All	3015	0	2788	17	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 3.

All (17) 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:325:THR:HG21	1:A:353:PRO:HB3	1.63	0.80
1:A:417:HIS:HD2	1:A:419:ASN:H	1.45	0.63
1:A:296:THR:HA	1:A:299:GLN:HG2	1.82	0.61
1:A:417:HIS:HD2	1:A:420:ILE:H	1.49	0.58
1:A:409:LYS:HE2	1:A:463:LEU:HD22	1.86	0.58
1:A:235:PRO:HG2	1:A:238:ILE:HG12	1.85	0.58
1:A:417:HIS:CD2	1:A:419:ASN:H	2.22	0.57
1:A:417:HIS:CD2	1:A:420:ILE:H	2.24	0.54
1:A:356:MET:HG2	1:A:431:GLU:HB2	1.91	0.52
1:A:239:GLU:HB2	1:A:290:PHE:CZ	2.45	0.52
1:A:251:GLY:HA3	3:A:496:HOH:O	2.14	0.48
1:A:380:VAL:O	1:A:388:VAL:HG21	2.14	0.47
1:A:358:GLN:HE21	1:A:430:ASN:HD21	1.63	0.46
1:A:315:VAL:HG12	1:A:329:PRO:HG3	1.99	0.45
1:A:326:LYS:NZ	1:A:431:GLU:HG3	2.34	0.43
1:A:427:SER:OG	1:A:437:VAL:HG21	2.19	0.42
1:A:236:LEU:HD21	1:A:280:GLU:HG2	2.02	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	357/361 (99%)	351 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	311/314 (99%)	290 (93%)	21 (7%)	16	21

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	GLU
1	A	128	LEU
1	A	157	VAL
1	A	164	VAL
1	A	173	LEU
1	A	265	VAL
1	A	315	VAL
1	A	316	ARG
1	A	317	LEU
1	A	367	GLN
1	A	379	ASP
1	A	380	VAL
1	A	389	PHE
1	A	396[A]	TRP
1	A	396[B]	TRP
1	A	402	GLN
1	A	431	GLU
1	A	433	GLU
1	A	453	THR
1	A	464	ASP
1	A	471	GLU

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	233	GLN
1	A	274	ASN
1	A	358	GLN
1	A	402	GLN
1	A	417	HIS

### 5.3.3 RNA

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](#)

1 ligand is 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	D1D	A	2815	-	6,8,8	0.42	0	6,10,10	1.32	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	D1D	A	2815	-	-	-	0/0/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	358/361 (99%)	-0.09	4 (1%) 80 85	25, 54, 91, 115	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	120	HIS	2.9
1	A	396[A]	TRP	2.7
1	A	119	HIS	2.3
1	A	249	PHE	2.1

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	D1D	A	2815	8/8	0.92	0.15	53,53,54,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.