



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:13 PM GMT

PDB ID : 2C1Y  
Title : STRUCTURE OF PDI-RELATED CHAPERONE, WIND MUTANT-Y55K  
Authors : Sevvana, M.; Ma, Q.; Barnewitz, K.; Guo, C.; Soling, H.-D.; Ferrari, D.M.;  
Sheldrick, G.M.  
Deposited on : 2005-09-22  
Resolution : 2.25 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

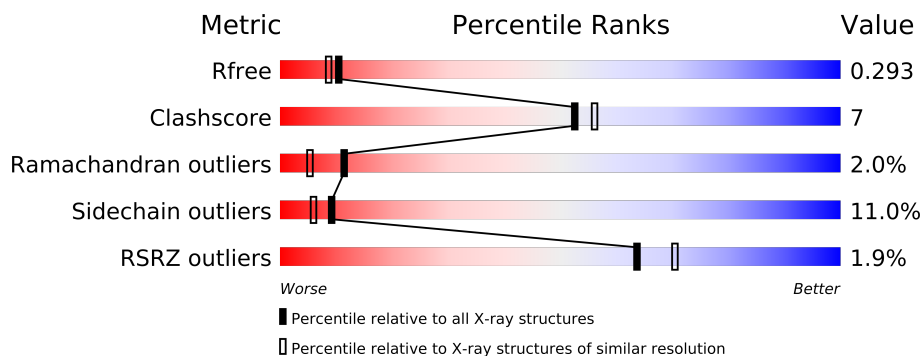
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.25 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))
$R_{free}$	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	248	
1	B	248	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2704 atoms, of which 0 are hydrogen and 0 are deuterium.

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 WINDBEUTEL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1720	1108	282	326	4			
1	B	128	Total	C	N	O	S	0	0	0
			929	596	153	178	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	LYS	TYR	ENGINEERED MUTATION	UNP O44342
B	55	LYS	TYR	ENGINEERED MUTATION	UNP O44342

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	35	Total	O	0	0
			35	35		
2	B	20	Total	O	0	0
			20	20		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	35.42Å 119.09Å 64.03Å 90.00° 100.53° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 59.55 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.25) 97.7 (59.55-2.25)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.223 , 0.292 0.226 , 0.293	Depositor DCC
$R_{free}$ test set	1220 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 24201 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2704	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	1.52	17/1751 (1.0%)	1.37	19/2377 (0.8%)
1	B	1.58	7/950 (0.7%)	1.39	11/1293 (0.9%)
All	All	1.54	24/2701 (0.9%)	1.37	30/3670 (0.8%)

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	2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	GLU	CG-CD	8.75	1.65	1.51
1	A	32	GLU	CB-CG	7.88	1.67	1.52
1	A	81	VAL	CB-CG1	7.43	1.68	1.52
1	B	40	GLU	CB-CG	7.23	1.65	1.52
1	A	143	TYR	CD2-CE2	7.01	1.49	1.39
1	A	184	ASP	CB-CG	6.98	1.66	1.51
1	A	173	GLU	CB-CG	6.75	1.65	1.52
1	A	203	GLU	CG-CD	6.59	1.61	1.51
1	A	246	LYS	C-O	6.55	1.35	1.23
1	A	119	VAL	CB-CG2	-6.14	1.40	1.52
1	A	118	TYR	C-O	6.04	1.34	1.23
1	A	149	CYS	CB-SG	6.02	1.92	1.82
1	A	79	ALA	CA-CB	5.96	1.65	1.52
1	A	194	TYR	CD1-CE1	5.80	1.48	1.39
1	B	81	VAL	CB-CG2	5.72	1.64	1.52
1	B	134	ALA	CA-CB	5.71	1.64	1.52
1	B	53	TYR	N-CA	5.41	1.57	1.46
1	A	241	VAL	CA-CB	5.25	1.65	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	GLU	CG-CD	5.23	1.59	1.51
1	A	62	PHE	CD2-CE2	5.21	1.49	1.39
1	A	97	ARG	NE-CZ	5.14	1.39	1.33
1	B	144	ILE	CA-C	5.13	1.66	1.52
1	B	40	GLU	CD-OE1	5.11	1.31	1.25
1	B	136	VAL	CA-CB	5.04	1.65	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ARG	NE-CZ-NH2	-12.79	113.91	120.30
1	A	218	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	A	41	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	50	ASP	CB-CG-OD1	7.58	125.13	118.30
1	A	184	ASP	CB-CG-OD1	7.35	124.92	118.30
1	B	77	LEU	CA-CB-CG	6.92	131.22	115.30
1	A	209	LEU	CA-CB-CG	6.87	131.10	115.30
1	A	41	ARG	CG-CD-NE	-6.87	97.38	111.80
1	A	130	ASP	CB-CG-OD1	6.57	124.22	118.30
1	A	119	VAL	CG1-CB-CG2	-6.52	100.47	110.90
1	B	29	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	50	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	116	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	76	LEU	CA-CB-CG	6.33	129.87	115.30
1	A	252	PRO	N-CA-C	6.13	128.05	112.10
1	A	130	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	B	22	VAL	N-CA-C	5.92	126.99	111.00
1	B	29	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	132	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	50	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	B	31	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	165	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	86	TYR	N-CA-C	-5.44	96.31	111.00
1	B	81	VAL	N-CA-C	-5.37	96.49	111.00
1	B	144	ILE	CB-CA-C	5.37	122.35	111.60
1	A	110	LEU	CA-CB-CG	5.26	127.40	115.30
1	B	77	LEU	CB-CG-CD2	5.19	119.82	111.00
1	A	173	GLU	CA-CB-CG	5.11	124.64	113.40
1	B	130	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	A	41	ARG	CB-CA-C	-5.08	100.24	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	ALA	Peptide
1	A	85	ASP	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1720	0	14	17	0
1	B	929	0	18	2	0
2	A	35	0	0	6	0
2	B	20	0	0	1	0
All	All	2704	0	32	19	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (19) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:252:PRO:CB	2:A:2034:HOH:O	1.64	1.32
1:A:97:ARG:CG	2:A:2014:HOH:O	2.18	0.90
1:A:97:ARG:NE	2:A:2014:HOH:O	2.12	0.82
1:A:252:PRO:N	2:A:2033:HOH:O	2.12	0.81
1:A:97:ARG:CD	2:A:2014:HOH:O	2.35	0.75
1:B:133:LYS:NZ	1:B:145:GLY:O	2.23	0.72
1:A:23:THR:O	1:A:24:CYS:O	2.14	0.64
1:B:149:CYS:C	2:B:2020:HOH:O	2.39	0.60
1:A:207:ASP:N	1:A:207:ASP:OD1	2.38	0.56
1:A:100:VAL:O	1:A:100:VAL:CG2	2.58	0.52
1:A:102:ASP:OD2	1:A:102:ASP:N	2.43	0.51
1:A:97:ARG:NH2	1:A:116:ASP:OD1	2.49	0.45
1:A:204:VAL:CG1	1:A:204:VAL:O	2.66	0.44
1:A:23:THR:O	1:A:23:THR:OG1	2.34	0.44
1:A:210:GLU:O	1:A:214:LYS:CG	2.65	0.43
1:A:97:ARG:NH1	2:A:2015:HOH:O	2.52	0.43
1:A:121:LEU:O	1:A:122:PRO:C	2.55	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:159:ASN:O	1:A:163:ILE:CG2	2.69	0.41
1:A:53:TYR:N	1:A:54:PRO:CD	2.84	0.40

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	229/248 (92%)	211 (92%)	13 (6%)	5 (2%)	10	4
1	B	126/248 (51%)	116 (92%)	8 (6%)	2 (2%)	14	8
All	All	355/496 (72%)	327 (92%)	21 (6%)	7 (2%)	11	5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	CYS
1	A	104	ASN
1	A	252	PRO
1	B	144	ILE
1	A	185	PRO
1	B	146	ARG
1	A	53	TYR

### 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	164/218 (75%)	145 (88%)	19 (12%)	8	5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	90/218 (41%)	81 (90%)	9 (10%)	11	7
All	All	254/436 (58%)	226 (89%)	28 (11%)	9	6

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	55	LYS
1	A	84	LYS
1	A	85	ASP
1	A	89	LEU
1	A	97	ARG
1	A	102	ASP
1	A	126	ASP
1	A	129	LEU
1	A	130	ASP
1	A	132	LEU
1	A	159	ASN
1	A	163	ILE
1	A	184	ASP
1	A	185	PRO
1	A	187	GLN
1	A	207	ASP
1	A	248	THR
1	A	250	THR
1	B	24	CYS
1	B	71	LYS
1	B	77	LEU
1	B	102	ASP
1	B	105	PHE
1	B	112	LYS
1	B	129	LEU
1	B	130	ASP
1	B	132	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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 ⓘ

### 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<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	231/248 (93%)	0.17	7 (3%) 48 55	30, 47, 75, 96	0
1	B	128/248 (51%)	0.18	0 100 100	29, 46, 69, 75	0
All	All	359/496 (72%)	0.17	7 (1%) 64 70	29, 47, 73, 96	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	LEU	3.3
1	A	143	TYR	3.0
1	A	135	PHE	2.5
1	A	247	VAL	2.4
1	A	182	LEU	2.2
1	A	202	HIS	2.0
1	A	68	SER	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.