

wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2024 – 10:15 AM EDT

:	8UC5
:	Apo X-ray crystal structure of Cyclophilin D with a surface entropy reduction
	mutation (K175I)
:	Kreitler, D.F.; Rangwala, A.M.; Seeliger, M.A.
	2023-09-25
:	1.43 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 (1)) were used in the production of this report:

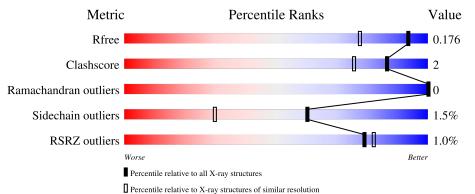
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as 543 be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.43 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	164625	2809 (1.46-1.42)
Clashscore	180529	3008 (1.46-1.42)
Ramachandran outliers	177936	2971 (1.46-1.42)
Sidechain outliers	177891	2971 (1.46-1.42)
RSRZ outliers	164620	2809 (1.46-1.42)

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	А	166	% 95%	•••
1	В	166	% 93%	5% ••
1	Х	166	% 96%	•••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMS	А	201	-	-	Х	-
2	DMS	Х	206	-	Х	-	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4190 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	x	165	Total	С	Ν	0	\mathbf{S}	0	4	0
1	Λ	105	1274	806	223	238	3 7 0		4	0
1	٨	165	Total	С	Ν	0	S	0	3	0
	Л	105	1264	802	220	235	7	0		0
1	р	165	Total	С	Ν	0	S	0	2	0
	ГВ	B 165	1254	796	217	234	$\overline{7}$	0		U

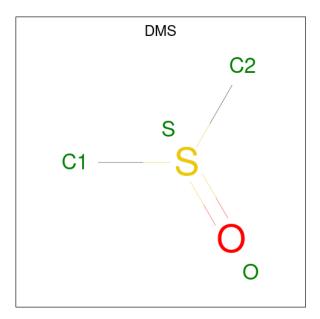
• Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase F, mitochondrial.

Chain	Residue	Modelled	Actual	Comment	Reference
Х	0	SER	-	expression tag	UNP P30405
Х	1	ASN	-	expression tag	UNP P30405
Х	2	ALA	-	expression tag	UNP P30405
Х	133	ILE	LYS	engineered mutation	UNP P30405
А	0	SER	-	expression tag	UNP P30405
А	1	ASN	-	expression tag	UNP P30405
А	2	ALA	-	expression tag	UNP P30405
А	133	ILE	LYS	engineered mutation	UNP P30405
В	0	SER	-	expression tag	UNP P30405
В	1	ASN	-	expression tag	UNP P30405
В	2	ALA	-	expression tag	UNP P30405
В	133	ILE	LYS	engineered mutation	UNP P30405

There are 12 discrepancies between the modelled and reference sequences:

• Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
2	X	1	Total	С	0	S	0	0
			4 Tatal	$\frac{2}{C}$	$\frac{1}{0}$	$\frac{1}{\mathrm{S}}$		
2	Х	1	Total 4	$\frac{0}{2}$	1	5 1	0	0
0	v	1	Total	Ē	0	S	0	0
2	Х	1	4	2	1	1	0	0
2	X	1	Total	С	0	\mathbf{S}	0	0
	Λ	1	4	2	1	1	0	0
2	X	1	Total	С	0	S	0	0
		_	4	2	1	1		
2	Х	1	Total	С	0	S	0	0
			4	2	1	1		
2	А	1	Total	С	0	S	0	0
			4	2	1	1		
2	А	1	Total	С	0	S	0	0
			4	2	1	1		
2	А	1	Total	С	0	S	0	0
			4	2	1	1		-
2	В	1	Total	С	0	S	0	0
	-	-	4	2	1	1	, č	, , , , , , , , , , , , , , , , , , ,
2	В	1	Total	С	0	\mathbf{S}	0	0
_	2	÷	4	2	1	1	Ŭ	Ŭ

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Х	1	Total 1	Na 1	0	0
				ž		next page

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Na 1 1	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Х	2	Total Cl 2 2	0	0
4	А	1	Total Cl 1 1	0	0

• Molecule 5 is water.

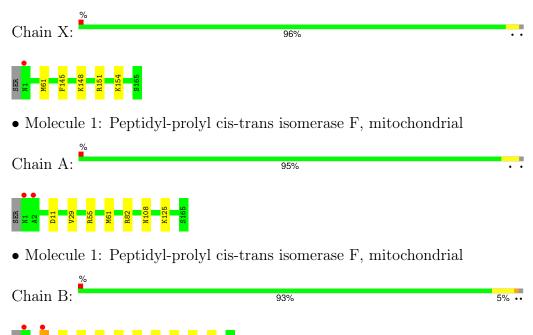
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Х	137	Total O 137 137	0	0
5	А	119	Total O 119 119	0	0
5	В	93	Total O 93 93	0	0



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: Peptidyl-prolyl cis-trans isomerase F, mitochondrial





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	123.67Å 56.64Å 101.17Å	Depositor
a, b, c, α , β , γ	90.00° 123.72° 90.00°	Depositor
Resolution (Å)	29.33 - 1.43	Depositor
Resolution (A)	29.33 - 1.43	EDS
% Data completeness	97.4 (29.33-1.43)	Depositor
(in resolution range)	97.6 (29.33-1.43)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.12 (at 1.43 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18rc7_3834	Depositor
D D.	0.144 , 0.175	Depositor
R, R_{free}	0.144 , 0.176	DCC
R_{free} test set	105616 reflections $(1.90%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	15.2	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.44,51.0	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4190	wwPDB-VP
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.61% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: NA, CL, DMS

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.52	0/1298	0.69	1/1749~(0.1%)	
1	В	0.49	0/1287	0.67	0/1734	
1	Х	0.54	0/1307	0.68	0/1760	
All	All	0.52	0/3892	0.68	1/5243~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	11	ASP	CB-CA-C	-5.42	99.57	110.40

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	А	1264	0	1258	5	0
1	В	1254	0	1252	6	0
1	Х	1274	0	1272	3	0
2	А	12	0	18	4	0
2	В	8	0	12	3	0
2	Х	24	0	36	0	0
3	А	1	0	0	0	0

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	Chain	-	- 0	H(added) Clashes		Symm-Clashes
3	Х	1	0	0	0	0
4	А	1	0	0	1	0
4	Х	2	0	0	1	0
5	А	119	0	0	1	0
5	В	93	0	0	0	0
5	Х	137	0	0	1	0
All	All	4190	0	3848	15	0

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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 2.

The worst 5 of 15 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:B:55:ARG:HH12	2:B:201:DMS:H22	1.56	0.71
1:B:55:ARG:HH12	2:B:201:DMS:C2	2.05	0.69
1:A:55:ARG:HH12	2:A:201:DMS:C1	2.11	0.64
2:A:201:DMS:H11	5:A:409:HOH:O	2.01	0.59
5:X:427:HOH:O	2:B:201:DMS:H23	2.06	0.54

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	Perce	ntiles
1	А	166/166~(100%)	160 (96%)	6~(4%)	0	100	100
1	В	165/166~(99%)	159 (96%)	6 (4%)	0	100	100
1	Х	167/166~(101%)	162 (97%)	5(3%)	0	100	100
All	All	498/498 (100%)	481 (97%)	17 (3%)	0	100	100



There are no Ramachandran outliers to report.

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	Rotameric Outliers		tiles
1	А	138/137~(101%)	136~(99%)	2(1%)	62	32
1	В	137/137~(100%)	134~(98%)	3~(2%)	47	14
1	Х	140/137~(102%)	139~(99%)	1 (1%)	81 6	61
All	All	415/411 (101%)	409 (99%)	6 (1%)	60	32

5 of 6 residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type	
1	В	11	ASP	
1	В	29	VAL	
1	В	61	MET	
1	А	29	VAL	
1	Х	61	MET	

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

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 oligosaccharides in this entry.



5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 for Mogul analysis.

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	Turne	Chain	Dec	Link	B	ond leng	gths	I	Bond an	gles
INIOI	Type	Unam	Res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	Х	205	-	$3,\!3,\!3$	0.61	0	$3,\!3,\!3$	0.39	0
2	DMS	Х	201	-	3,3,3	0.61	0	$3,\!3,\!3$	0.33	0
2	DMS	А	203	-	3, 3, 3	0.70	0	$3,\!3,\!3$	0.43	0
2	DMS	В	202	-	3, 3, 3	0.77	0	$3,\!3,\!3$	0.45	0
2	DMS	Х	202	-	3, 3, 3	0.67	0	$3,\!3,\!3$	0.79	0
2	DMS	Х	204	-	3, 3, 3	0.61	0	$3,\!3,\!3$	0.91	0
2	DMS	В	201	-	$3,\!3,\!3$	0.55	0	$3,\!3,\!3$	0.46	0
2	DMS	А	202	-	3, 3, 3	0.61	0	$3,\!3,\!3$	0.96	0
2	DMS	А	201	-	$3,\!3,\!3$	0.68	0	$3,\!3,\!3$	0.82	0
2	DMS	Х	203	-	3, 3, 3	0.70	0	$3,\!3,\!3$	0.48	0
2	DMS	Х	206	-	$3,\!3,\!3$	0.39	0	$3,\!3,\!3$	<mark>3.13</mark>	3 (100%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Х	206	DMS	O-S-C1	3.60	124.50	106.49
2	Х	206	DMS	O-S-C2	3.34	123.19	106.49
2	Х	206	DMS	C2-S-C1	2.29	110.15	98.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

ſ	Mol	Chain	Res	Type	Clashes	Symm-Clashes
	2	В	201	DMS	3	0
	2	А	201	DMS	4	0



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, 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	А	165/166~(99%)	-0.63	2 (1%) 76 79	8, 15, 24, 38	3 (1%)
1	В	165/166~(99%)	-0.31	2 (1%) 76 79	13, 20, 31, 40	2 (1%)
1	Х	165/166~(99%)	-0.74	1 (0%) 85 88	6, 14, 21, 36	4 (2%)
All	All	495/498 (99%)	-0.56	5 (1%) 79 82	6, 16, 28, 40	9 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	1	ASN	3.8
1	А	1	ASN	3.6
1	В	11	ASP	3.4
1	Х	1	ASN	2.8
1	А	2	ALA	2.4

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 monosaccharides 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^{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.



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors($Å^2$)	Q<0.9
2	DMS	Х	206	4/4	0.76	0.25	45,45,47,51	0
2	DMS	Х	203	4/4	0.88	0.20	43,51,51,52	0
2	DMS	Х	204	4/4	0.90	0.18	45,45,46,47	0
2	DMS	Х	202	4/4	0.90	0.22	49,53,53,53	0
3	NA	А	204	1/1	0.92	0.17	30,30,30,30	0
2	DMS	В	202	4/4	0.93	0.15	$30,\!36,\!36,\!37$	0
2	DMS	А	202	4/4	0.94	0.13	37,37,39,43	0
4	CL	Х	208	1/1	0.96	0.13	$35,\!35,\!35,\!35$	0
3	NA	Х	207	1/1	0.97	0.09	30,30,30,30	0
2	DMS	В	201	4/4	0.97	0.09	22,22,25,27	0
2	DMS	А	201	4/4	0.97	0.10	$26,\!26,\!28,\!28$	0
2	DMS	А	203	4/4	0.98	0.14	22,24,25,25	0
2	DMS	Х	205	4/4	0.99	0.09	21,22,24,28	0
2	DMS	Х	201	4/4	0.99	0.08	21,22,22,23	0
4	CL	Х	209	1/1	0.99	0.09	29,29,29,29	0
4	CL	А	205	1/1	0.99	0.11	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.

