



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 10:19 pm BST

PDB ID : 1VBS
Title : STRUCTURE OF CYCLOPHILIN COMPLEXED WITH (D)ALA CONTAINING TETRAPEPTIDE
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Deposited on : 1998-06-16
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

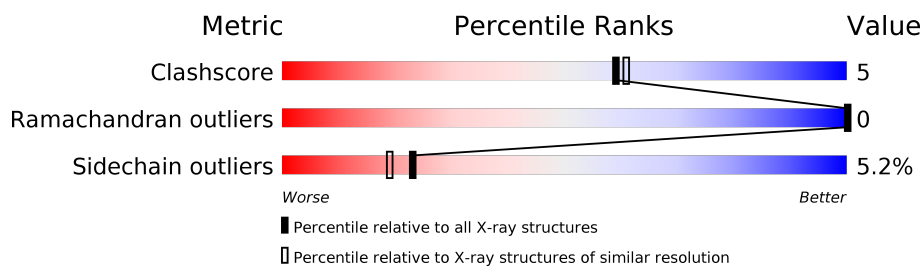
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	165	
2	B	5	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1852 atoms, of which 467 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 CYCLOPHILIN A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	164	Total	C	H	N	O	S	0	0	0
			1541	797	283	217	236	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P05092

- Molecule 2 is a protein called TETRAPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	5	Total	C	H	N	O	0	0	0
			44	26	6	6	6			

- Molecule 3 is water.


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	81	Total	H	O	0	0
			243	162	81		
3	B	8	Total	H	O	0	0
			24	16	8		

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. 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. 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.

Note EDS was not executed.

- Molecule 1: CYCLOPHILIN A

Chain A: 



- Molecule 2: TETRAPEPTIDE

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 3 ₂ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	67.10 Å 67.10 Å 95.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	88.0 (10.00-2.00)	Depositor
R _{merge}	0.09	Depositor
R _{sym}	0.09	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R _{free}	0.198 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1852	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.60	0/1286	0.74	0/1723
2	B	0.73	0/23	0.97	0/28
All	All	0.60	0/1309	0.74	0/1751

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

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	1258	283	1225	11	0
2	B	38	6	30	1	0
3	A	81	162	0	0	0
3	B	8	16	0	0	0
All	All	1385	467	1255	12	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 5.

All (12) 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:5:THR:HB	1:A:165:GLU:HG2	1.53	0.90
1:A:147:SER:OG	1:A:151:LYS:HD3	1.98	0.64
1:A:52:CYS:HB3	1:A:155:LYS:NZ	2.17	0.60
1:A:82:LYS:HA	1:A:108:ASN:O	2.03	0.58
1:A:56:ILE:O	1:A:150:GLY:HA2	2.06	0.55
1:A:25:PHE:CD2	1:A:90:LEU:HD13	2.43	0.53
1:A:145:PHE:HB2	1:A:156:ILE:HD11	1.94	0.50
1:A:5:THR:CB	1:A:165:GLU:HG2	2.38	0.44
1:A:52:CYS:HB3	1:A:155:LYS:HZ1	1.84	0.43
1:A:69:ARG:HD3	1:A:69:ARG:HA	1.82	0.41
1:A:119:THR:HA	1:A:121:TRP:CZ3	2.55	0.41
2:B:5:PHE:O	2:B:6:NIT:H6	2.20	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	162/165 (98%)	156 (96%)	6 (4%)	0	100	100
2	B	1/5 (20%)	1 (100%)	0	0	100	100
All	All	163/170 (96%)	157 (96%)	6 (4%)	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	Outliers	Percentiles	
1	A	132/133 (99%)	125 (95%)	7 (5%)	22	18
2	B	2/2 (100%)	2 (100%)	0	100	100
All	All	134/135 (99%)	127 (95%)	7 (5%)	23	19

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	15	GLU
1	A	29	VAL
1	A	61	MET
1	A	84	GLU
1	A	151	LYS
1	A	155	LYS

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 molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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.

5.5 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.