



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:41 pm BST

PDB ID : 1IIP  
Title : Bovine Cyclophilin 40, Tetragonal Form  
Authors : Taylor, P.; Dornan, J.; Carrello, A.; Minchin, R.F.; Ratajczak, T.; Walkinshaw, M.D.  
Deposited on : 2001-04-24  
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](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)  
Xtrriage (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

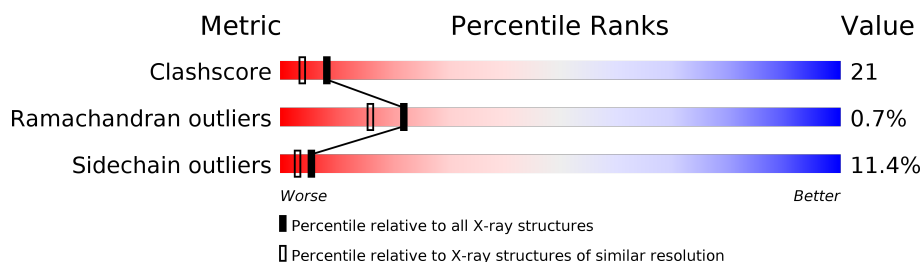
# 1 Overall quality at a glance

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  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	370	

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	GOL	A	371	-	-	X	-

## 2 Entry composition [i](#)

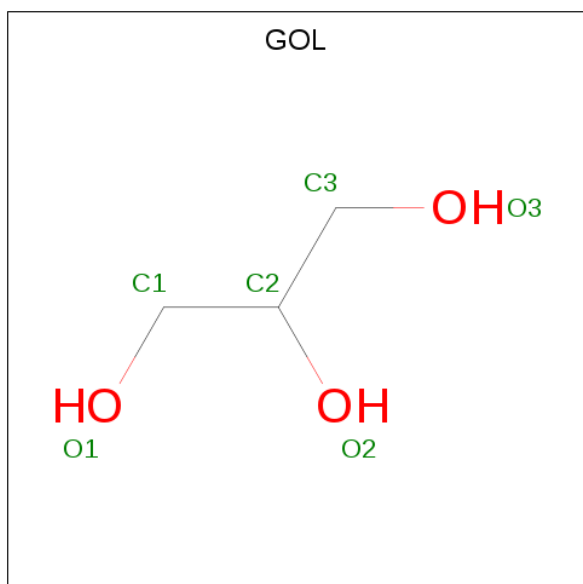
There are 3 unique types of molecules in this entry. The entry contains 2493 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cyclophilin 40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2275	1439	387	437	12	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0

- Molecule 3 is water.

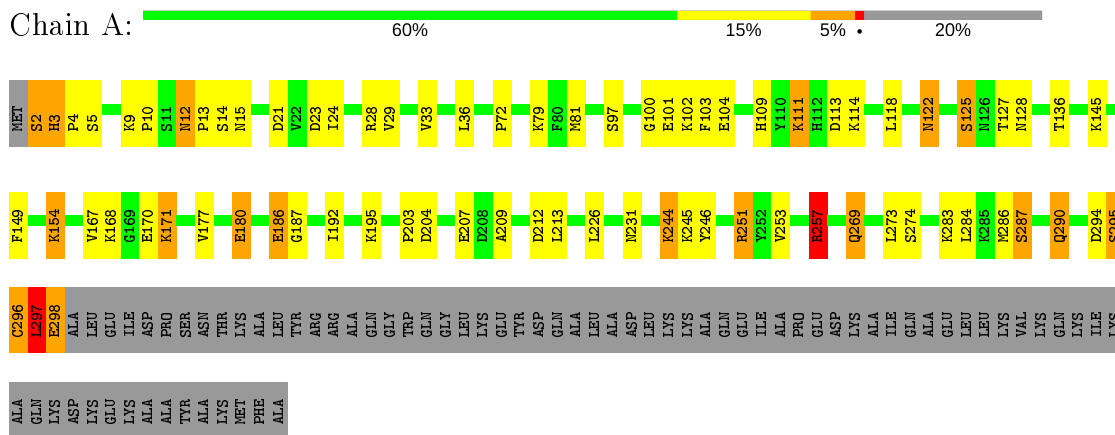
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	212	212	212	0	0

### 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 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 40



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.58Å 94.58Å 118.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.00 – 2.00	Depositor
% Data completeness (in resolution range)	87.1 (24.00-2.00)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.236 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2493	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

## 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: GOL

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	0.34	0/2325	1.06	6/3135 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	257	ARG	NE-CZ-NH1	15.31	127.95	120.30
1	A	251	ARG	CD-NE-CZ	14.00	143.20	123.60
1	A	251	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	A	257	ARG	CD-NE-CZ	10.05	137.67	123.60
1	A	251	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	A	257	ARG	NE-CZ-NH2	-7.42	116.59	120.30

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	2275	0	2234	95	0
2	A	6	0	8	5	0
3	A	212	0	0	19	2
All	All	2493	0	2242	95	2

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 21.

All (95) 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:4:PRO:HA	1:A:111:LYS:HD2	1.23	1.17
1:A:111:LYS:CG	1:A:113:ASP:HB3	1.90	1.01
1:A:294:ASP:O	1:A:298:GLU:HB3	1.62	0.99
1:A:101:GLU:HG2	1:A:102:LYS:HD3	1.46	0.97
1:A:111:LYS:HG3	1:A:113:ASP:HB3	1.46	0.94
1:A:297:LEU:C	1:A:297:LEU:CD1	2.35	0.94
1:A:297:LEU:C	1:A:297:LEU:HD13	1.90	0.92
1:A:251:ARG:HH12	2:A:371:GOL:C1	1.82	0.91
1:A:269:GLN:OE1	1:A:269:GLN:HA	1.72	0.90
1:A:154:LYS:HG2	1:A:192:ILE:HD13	1.57	0.86
1:A:195:LYS:HB3	3:A:592:HOH:O	1.76	0.86
1:A:3:HIS:CD2	1:A:3:HIS:N	2.44	0.85
1:A:186:GLU:OE1	1:A:187:GLY:N	2.11	0.84
1:A:251:ARG:HH12	2:A:371:GOL:H12	1.44	0.81
1:A:287:SER:O	1:A:290:GLN:HG3	1.81	0.81
1:A:4:PRO:CA	1:A:111:LYS:HD2	2.12	0.76
1:A:297:LEU:HD13	1:A:297:LEU:O	1.84	0.75
1:A:204:ASP:OD1	3:A:431:HOH:O	2.05	0.75
1:A:101:GLU:HG2	1:A:102:LYS:CD	2.19	0.73
1:A:251:ARG:NH1	2:A:371:GOL:C1	2.52	0.73
1:A:101:GLU:OE2	1:A:102:LYS:HG2	1.93	0.69
1:A:251:ARG:NH1	2:A:371:GOL:H11	2.08	0.68
1:A:12:ASN:HD22	1:A:13:PRO:CD	2.07	0.68
1:A:5:SER:OG	1:A:114:LYS:HE3	1.93	0.67
1:A:12:ASN:HD22	1:A:13:PRO:HD2	1.59	0.67
1:A:102:LYS:CE	3:A:547:HOH:O	2.42	0.67
1:A:101:GLU:OE2	1:A:102:LYS:CE	2.43	0.66
1:A:136:THR:HB	3:A:523:HOH:O	1.94	0.66
1:A:297:LEU:HD12	1:A:298:GLU:N	2.10	0.66
1:A:297:LEU:C	1:A:297:LEU:HD12	2.17	0.65
1:A:101:GLU:OE2	1:A:102:LYS:CG	2.45	0.64
1:A:100:GLY:HA3	3:A:589:HOH:O	1.97	0.64
1:A:296:CYS:C	1:A:298:GLU:H	1.99	0.64
1:A:24:ILE:HD12	1:A:29:VAL:HG21	1.79	0.64
1:A:2:SER:C	1:A:3:HIS:CD2	2.72	0.63
1:A:104:GLU:OE1	1:A:104:GLU:N	2.25	0.63
1:A:167:VAL:HG21	1:A:170:GLU:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASN:HD22	1:A:13:PRO:N	1.98	0.61
1:A:294:ASP:O	1:A:297:LEU:HD12	2.00	0.61
1:A:111:LYS:CD	1:A:113:ASP:HB3	2.30	0.60
1:A:3:HIS:HD2	1:A:3:HIS:N	1.97	0.60
1:A:113:ASP:OD2	3:A:468:HOH:O	2.17	0.59
1:A:167:VAL:HG23	1:A:171:LYS:C	2.22	0.58
1:A:296:CYS:C	1:A:298:GLU:N	2.57	0.58
1:A:251:ARG:NH1	2:A:371:GOL:H12	2.17	0.57
1:A:295:SER:HA	1:A:298:GLU:CD	2.24	0.57
1:A:12:ASN:HD22	1:A:12:ASN:C	2.07	0.57
1:A:101:GLU:C	1:A:102:LYS:HD3	2.26	0.56
1:A:167:VAL:HG23	1:A:171:LYS:O	2.05	0.55
1:A:167:VAL:HG21	1:A:170:GLU:CA	2.37	0.55
1:A:203:PRO:HG2	1:A:209:ALA:HA	1.89	0.55
1:A:212:ASP:HB2	3:A:575:HOH:O	2.08	0.54
1:A:244:LYS:HE2	3:A:443:HOH:O	2.07	0.53
1:A:72:PRO:HA	1:A:177:VAL:HA	1.90	0.53
1:A:21:ASP:HB2	1:A:180:GLU:HG3	1.91	0.53
1:A:195:LYS:CA	3:A:592:HOH:O	2.56	0.53
1:A:296:CYS:O	1:A:298:GLU:N	2.41	0.53
1:A:79:LYS:HE3	1:A:79:LYS:HA	1.89	0.52
1:A:12:ASN:ND2	1:A:13:PRO:HD2	2.24	0.52
1:A:23:ASP:OD1	1:A:28:ARG:HA	2.10	0.52
1:A:207:GLU:HG3	3:A:551:HOH:O	2.10	0.51
1:A:33:VAL:HB	1:A:154:LYS:HB2	1.92	0.51
1:A:253:VAL:O	1:A:257:ARG:HG3	2.11	0.51
1:A:167:VAL:CG2	1:A:170:GLU:C	2.80	0.50
1:A:297:LEU:CD1	1:A:298:GLU:N	2.70	0.49
1:A:15:ASN:HB3	1:A:36:LEU:O	2.13	0.49
1:A:102:LYS:HA	1:A:128:ASN:O	2.13	0.48
1:A:101:GLU:CD	1:A:102:LYS:HG2	2.34	0.48
1:A:111:LYS:HE3	1:A:111:LYS:HB3	1.65	0.48
1:A:3:HIS:CD2	1:A:109:HIS:O	2.66	0.48
1:A:12:ASN:ND2	1:A:14:SER:H	2.12	0.47
1:A:287:SER:OG	3:A:519:HOH:O	2.20	0.47
1:A:122:ASN:C	1:A:122:ASN:HD22	2.19	0.46
1:A:12:ASN:C	1:A:12:ASN:ND2	2.69	0.46
1:A:167:VAL:HG21	1:A:170:GLU:C	2.35	0.46
1:A:3:HIS:HD2	1:A:109:HIS:O	1.99	0.45
1:A:273:LEU:HD23	3:A:570:HOH:O	2.16	0.45
1:A:102:LYS:HE2	3:A:547:HOH:O	2.12	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:HIS:C	1:A:111:LYS:HE3	2.37	0.45
1:A:118:LEU:HG	1:A:149:PHE:CZ	2.51	0.44
1:A:125:SER:O	1:A:127:THR:HG23	2.18	0.44
1:A:102:LYS:NZ	3:A:547:HOH:O	2.51	0.43
1:A:23:ASP:OD1	1:A:28:ARG:NE	2.46	0.43
1:A:101:GLU:OE2	1:A:102:LYS:HE3	2.18	0.42
1:A:111:LYS:HD3	1:A:113:ASP:HB3	2.02	0.42
1:A:186:GLU:C	1:A:186:GLU:CD	2.77	0.42
1:A:231:ASN:ND2	1:A:246:TYR:OH	2.47	0.42
1:A:111:LYS:CG	1:A:113:ASP:CB	2.80	0.42
1:A:283:LYS:NZ	3:A:581:HOH:O	2.52	0.41
1:A:101:GLU:N	3:A:589:HOH:O	2.54	0.41
1:A:101:GLU:OE2	1:A:102:LYS:HE2	2.18	0.41
1:A:195:LYS:CB	3:A:592:HOH:O	2.47	0.41
1:A:9:LYS:HA	1:A:10:PRO:HA	1.81	0.41
1:A:114:LYS:NZ	3:A:507:HOH:O	2.52	0.41
1:A:286:MET:HE1	3:A:601:HOH:O	2.20	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:529:HOH:O	3:A:529:HOH:O[2_765]	1.96	0.24
3:A:524:HOH:O	3:A:560:HOH:O[5_755]	2.00	0.20

## 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	295/370 (80%)	286 (97%)	7 (2%)	2 (1%)	22 16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	CYS
1	A	297	LEU

### 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	246/303 (81%)	218 (89%)	28 (11%)	<b>5</b> <b>3</b>

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

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	HIS
1	A	12	ASN
1	A	81	MET
1	A	97	SER
1	A	103	PHE
1	A	111	LYS
1	A	122	ASN
1	A	125	SER
1	A	145	LYS
1	A	154	LYS
1	A	168	LYS
1	A	171	LYS
1	A	180	GLU
1	A	186	GLU
1	A	213	LEU
1	A	226	LEU
1	A	244	LYS
1	A	245	LYS
1	A	257	ARG
1	A	269	GLN
1	A	274	SER
1	A	284	LEU
1	A	287	SER
1	A	290	GLN

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Mol	Chain	Res	Type
1	A	295	SER
1	A	297	LEU
1	A	298	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	12	ASN
1	A	109	HIS
1	A	122	ASN
1	A	164	ASN
1	A	231	ASN
1	A	290	GLN

### 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](#)

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	GOL	A	371	-	5,5,5	0.57	0	5,5,5	0.67	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	GOL	A	371	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	371	GOL	O1-C1-C2-C3
2	A	371	GOL	C1-C2-C3-O3
2	A	371	GOL	O2-C2-C3-O3
2	A	371	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	371	GOL	5	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

### 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.