

# Full wwPDB X-ray Structure Validation Report (i)

### Feb 20, 2024 – 12:05 AM EST

PDB ID : 4LD3

Title : Structural analysis of the microcephaly protein CPAP G-box domain suggests

a role in centriole elongation.

Authors: Hatzopoulos, G.N.; Vakonakis, I.

Deposited on : 2013-06-24

Resolution : 2.44 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 (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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$ 

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

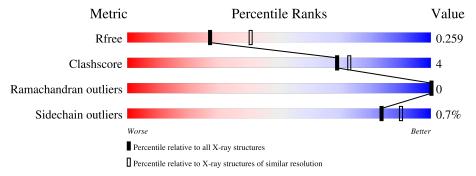
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	Similar resolution
Wiedite	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)

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%

Mol	Chain	Length	Quality of chain					
1	A	184		79%		5%	16%	
2	В	60	27%		73%	_		



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1383 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	154	Total 1239	C 775	N 217	O 244	S 3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	938	GLY	-	expression tag	UNP E7FCY1
A	939	PRO	-	expression tag	UNP E7FCY1
A	940	LEU	-	expression tag	UNP E7FCY1
A	941	GLY	-	expression tag	UNP E7FCY1

• Molecule 2 is a protein called SCL-interrupting locus protein homolog.

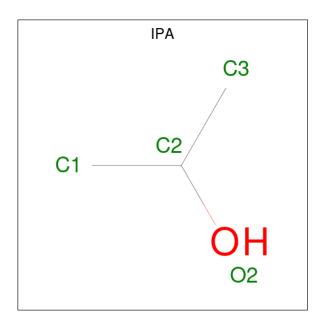
$\mathbf{Mol}$	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	В	16	Total 123		N 23	O 25	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	391	GLY	-	expression tag	UNP Q8JGS1
В	392	PRO	-	expression tag	UNP Q8JGS1
В	393	LEU	-	expression tag	UNP Q8JGS1
В	394	GLY	-	expression tag	UNP Q8JGS1
В	395	SER	-	expression tag	UNP Q8JGS1
В	396	CYS	-	expression tag	UNP Q8JGS1
В	397	TYR	-	expression tag	UNP Q8JGS1
В	398	GLN	-	expression tag	UNP Q8JGS1

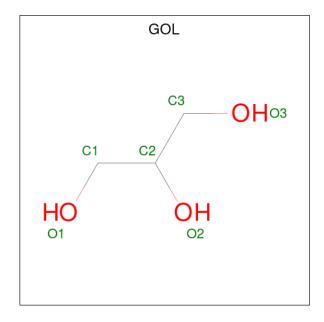
• Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 3 1	0	0
3	A	1	Total C O 4 3 1	0	0
3	A	1	Total C O 4 3 1	0	0

 $\bullet$  Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $\mathrm{C_3H_8O_3}).$ 



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total C C 6 3 3	)	0	0



## • Molecule 5 is water.

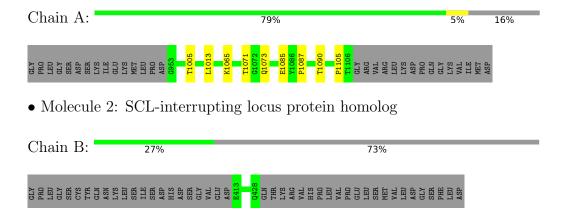
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	В	1	Total O 1 1	0	0



# 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. 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.

• Molecule 1: Uncharacterized protein





# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 32	Depositor	
Cell constants	79.40Å 79.40Å 50.56Å	Donositon	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor	
Resolution (Å)	28.87 - 2.44	Depositor	
rtesolution (A)	28.43 - 2.39	EDS	
% Data completeness	88.5 (28.87-2.44)	Depositor	
(in resolution range)	87.5 (28.43-2.39)	EDS	
$R_{merge}$	0.07	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.06  (at  2.39Å)	Xtriage	
Refinement program	BUSTER 2.10.0	Depositor	
$R, R_{free}$	0.198 , $0.214$	Depositor	
it, itfree	0.254 , $0.259$	DCC	
$R_{free}$ test set	613 reflections (4.98%)	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	62.8	Xtriage	
Anisotropy	1.187	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	$0.31 \; ,  72.2$	EDS	
L-test for twinning <sup>2</sup>	$< L > = 0.49, < L^2> = 0.32$	Xtriage	
	0.051 for -h,-k,l		
Estimated twinning fraction	0.062  for h,-h-k,-l	Xtriage	
	0.072  for -k,-h,-l		
$F_o, F_c$ correlation	0.94	EDS	
Total number of atoms	1383	wwPDB-VP	
Average B, all atoms $(\mathring{A}^2)$	113.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.

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



<sup>&</sup>lt;sup>1</sup>Intensities 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: GOL, IPA

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		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.50	0/1268	0.66	0/1719	
2	В	0.56	0/128	0.70	0/177	
All	All	0.50	0/1396	0.66	0/1896	

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 (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	1239	0	1188	10	0
2	В	123	0	113	0	0
3	A	12	0	23	2	0
4	A	6	0	8	0	0
5	A	2	0	0	0	0
5	В	1	0	0	1	0
All	All	1383	0	1332	10	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 4.

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic	Clash
		$\operatorname{distance}\left( \mathrm{\AA}\right)$	overlap (Å)
1:A:1090:THR:HG22	1:A:1105:PRO:HD3	1.28	1.14
1:A:1090:THR:CG2	1:A:1105:PRO:HD3	1.96	0.94
1:A:1065:LYS:HG2	3:A:1203:IPA:H12	1.62	0.81
1:A:1065:LYS:HG2	3:A:1203:IPA:C1	2.28	0.64
1:A:1071:THR:OG1	1:A:1073:GLN:HG2	1.98	0.62
1:A:1090:THR:HG22	1:A:1105:PRO:CD	2.17	0.58
1:A:1073:GLN:HB2	1:A:1085:GLU:O	2.05	0.57
1:A:1073:GLN:HE21	1:A:1087:PRO:HD3	1.76	0.51
1:A:1073:GLN:HB3	1:A:1087:PRO:HD3	1.99	0.45
1:A:1005:THR:HG23	5:B:501:HOH:O	2.17	0.44

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	A	152/184~(83%)	151 (99%)	1 (1%)	0	100	100
2	В	14/60 (23%)	13 (93%)	1 (7%)	0	100	100
All	All	166/244 (68%)	164 (99%)	2 (1%)	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	Analysed Rotameric Outliers		Percentiles
1	A	137/163 (84%)	136 (99%)	1 (1%)	84 90
2	В	16/56 (29%)	16 (100%)	0	100 100
All	All	153/219 (70%)	152 (99%)	1 (1%)	84 90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1013	LEU

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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

4 ligands are 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	В	ond leng	$_{ m gths}$	В	ond ang	gles
MIOI	туре	Cham	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	IPA	A	1201	-	3,3,3	0.74	0	3,3,3	0.82	0
3	IPA	A	1202	-	3,3,3	0.72	0	3,3,3	0.64	0



7	Mol	Trens	Chain	Dag	Link	В	ond leng	$_{ m gths}$	В	ond ang	gles
1	VIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
	4	GOL	A	1204	-	5,5,5	0.09	0	5,5,5	0.26	0
	3	IPA	A	1203	-	3,3,3	0.61	0	3,3,3	0.61	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.

$\mathbf{Mol}$	Type	Chain	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
4	GOL	A	1204	-	-	0/4/4/4	-

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1203	IPA	2	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

