

Full wwPDB X-ray Structure Validation Report (i)

Feb 20, 2024 – 12:47 PM EST

PDB ID	:	4LD1
Title	:	Structural analysis of the microcephaly protein CPAP G-box domain suggests
		a role in centrille elongation.
Authors	:	Hatzopoulos, G.N.; Vakonakis, I.
Deposited on	:	2013-06-24
Resolution	:	1.44 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:

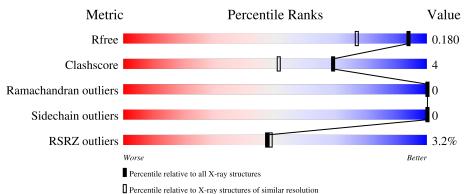
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.44 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (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	184	82%	•	15%



4LD1

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2928 atoms, of which 1346 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.

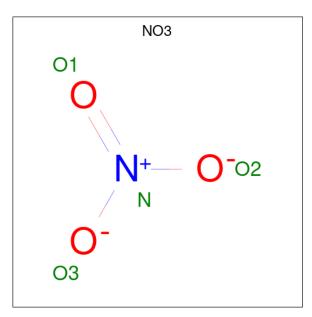
• Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	А	157	Total 2639	C 836	Н 1300	N 237	O 263	${ m S} { m 3}$	0	17	0

There are 4 discrepancies between the modelled and reference sequences:

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

• Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	А	1	Total 4	N 1	O 3	0	0

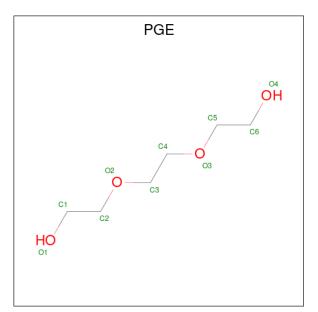
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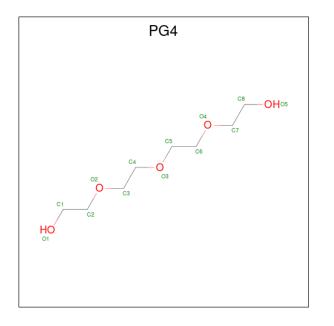
Mo	l Cha	in	Residues	Atoms			ZeroOcc	AltConf
2	А		1	Total 4	N 1	O 3	0	0

• Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	А	1	Total 24	C 6	Н 14	0 4	0	0

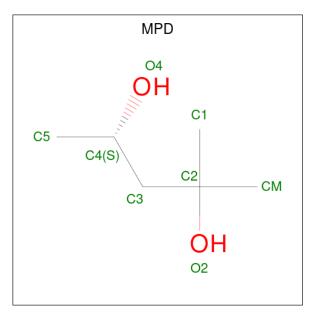
• Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	Λ	1	Total	С	Η	Ο	0	0
4	A	1	31	8	18	5	0	0

• Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	А	1	Total 22	C 6	H 14	O 2	0	0

• Molecule 6 is water.

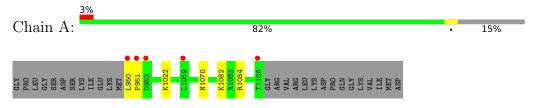
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	204	Total O 204 204	0	0



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: Uncharacterized protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	41.63Å 50.25Å 60.34Å	Deperitor
a, b, c, α , β , γ	90.00° 108.56° 90.00°	Depositor
Resolution (Å)	39.47 - 1.44	Depositor
Resolution (A)	39.47 - 1.44	EDS
% Data completeness	99.3 (39.47-1.44)	Depositor
(in resolution range)	99.3 (39.47 - 1.44)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.58 (at 1.44 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
D D	0.154 , 0.180	Depositor
R, R_{free}	0.155 , 0.180	DCC
R_{free} test set	2155 reflections $(5.06%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	22.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.41 , 48.1	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2928	wwPDB-VP
Average B, all atoms $(Å^2)$	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 9.36% 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: NO3, PG4, MPD, PGE

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).

Mal	Iol Bond lengths Dot Gal Dot Gal		Bond	angles	
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.47	0/1418	0.60	0/1920

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	А	1339	1300	1233	7	1
2	А	8	0	0	2	0
3	А	10	14	14	0	0
4	А	13	18	18	0	0
5	А	8	14	14	0	0
6	А	204	0	0	9	2
All	All	1582	1346	1279	10	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 4.

All (10) 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:950:LEU:N	6:A:1474:HOH:O	2.02	0.93
1:A:1022:LYS:NZ	6:A:1491:HOH:O	2.02	0.90
1:A:1082:LYS:NZ	6:A:1463:HOH:O	2.04	0.87
2:A:1205:NO3:O3	6:A:1439:HOH:O	2.04	0.74
2:A:1201:NO3:O1	6:A:1439:HOH:O	2.06	0.73
1:A:1070:ASN:ND2	6:A:1473:HOH:O	2.29	0.58
1:A:1084:ARG:NH1	6:A:1478:HOH:O	2.16	0.57
1:A:950:LEU:CA	6:A:1474:HOH:O	2.53	0.52
1:A:950:LEU:HB2	1:A:951:PRO:HD3	2.03	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)
6:A:1487:HOH:O	6:A:1490:HOH:O[2_445]	2.06	0.14
1:A:1022:LYS:NZ	6:A:1405:HOH:O[2_445]	2.17	0.03

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	Percer	ntiles
1	А	170/184~(92%)	169 (99%)	1 (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 Rotameric		Outliers	Perce	ntiles
1	А	155/163~(95%)	155 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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)

5 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	Trune	Chain	Res	Link	B	ond leng	gths	B	ond ang	les
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	NO3	А	1205	-	$1,\!3,\!3$	<mark>3.34</mark>	1 (100%)	0,3,3	-	-
5	MPD	А	1204	-	7,7,7	0.35	0	9,10,10	0.66	0
2	NO3	А	1201	-	$1,\!3,\!3$	3.40	1 (100%)	0,3,3	-	-
3	PGE	А	1202	-	9,9,9	0.33	0	8,8,8	0.28	0
4	PG4	А	1203	-	12,12,12	0.57	0	11,11,11	0.62	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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	А	1204	-	-	2/5/5/5	-
3	PGE	А	1202	-	-	4/7/7/7	-
4	PG4	А	1203	-	-	5/10/10/10	-

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

All (2) bond length outliers are listed below:

Mo	l Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	1201	NO3	O1-N	3.40	1.39	1.24
2	А	1205	NO3	O1-N	3.34	1.39	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	1203	PG4	C6-C5-O3-C4
3	А	1202	PGE	O1-C1-C2-O2
3	А	1202	PGE	O2-C3-C4-O3
3	А	1202	PGE	O3-C5-C6-O4
5	А	1204	MPD	C1-C2-C3-C4
4	А	1203	PG4	O3-C5-C6-O4
4	А	1203	PG4	O2-C3-C4-O3
4	А	1203	PG4	C4-C3-O2-C2
4	А	1203	PG4	C1-C2-O2-C3
3	А	1202	PGE	C4-C3-O2-C2
5	А	1204	MPD	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	1205	NO3	1	0
2	А	1201	NO3	1	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	$\langle RSRZ \rangle$	#RSRZ>2		$\mathbf{OWAB}(\mathbf{A}^2)$	Q < 0.9	
1	А	157/184~(85%)	0.00	5 (3%)	47	48	18, 29, 47, 71	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	951	PRO	6.1
1	А	952	ASP	4.3
1	А	950	LEU	3.6
1	А	1106	THR	2.4
1	А	1059	LEU	2.2

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	PG4	А	1203	13/13	0.83	0.21	$36,\!52,\!65,\!76$	0
5	MPD	А	1204	8/8	0.84	0.29	52,65,70,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	NO3	А	1205	4/4	0.85	0.21	40,43,51,61	0
3	PGE	А	1202	10/10	0.88	0.19	44,61,78,81	0
2	NO3	А	1201	4/4	0.93	0.13	50,53,60,63	0

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6.5 Other polymers (i)

There are no such residues in this entry.

