



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:28 PM GMT

PDB ID : 1P5U  
Title : X-ray structure of the ternary Caf1M:Caf1:Caf1 chaperone:subunit:subunit complex  
Authors : Zavialov, A.V.; Berglund, J.; Pudney, A.F.; Fooks, L.J.; Ibrahim, T.M.; MacIntyre, S.; Knight, S.D.  
Deposited on : 2003-04-28  
Resolution : 1.99 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

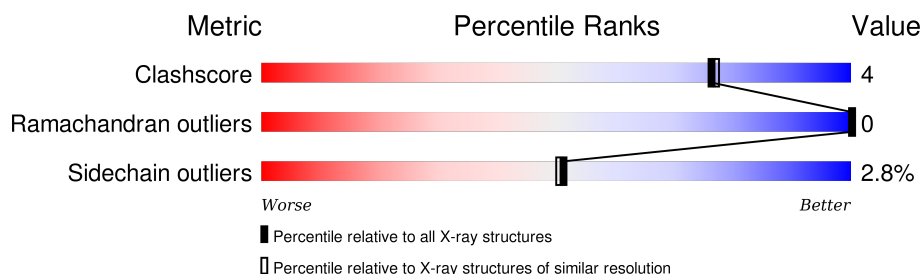
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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. 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	235	 71% 13% • 12%
2	B	149	 89% 10% •
3	C	147	 79% 8% • 12%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3982 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 Chaperone protein Caf1M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	4	0
			1627	1044	280	299	4			

- Molecule 2 is a protein called F1 capsule antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	149	Total	C	N	O	S	0	3	0
			1109	688	183	236	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	ARG	ALA	ENGINEERED	UNP P26948

- Molecule 3 is a protein called F1 capsule antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			956	595	158	201	2			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	ALA	-	EXPRESSION TAG	UNP P26948
C	4	ASP	-	EXPRESSION TAG	UNP P26948
C	5	LEU	-	EXPRESSION TAG	UNP P26948
C	6	THR	-	EXPRESSION TAG	UNP P26948
C	7	SER	-	EXPRESSION TAG	UNP P26948
C	8	HIS	-	EXPRESSION TAG	UNP P26948
C	9	HIS	-	EXPRESSION TAG	UNP P26948
C	10	HIS	-	EXPRESSION TAG	UNP P26948
C	11	HIS	-	EXPRESSION TAG	UNP P26948

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Chain	Residue	Modelled	Actual	Comment	Reference
C	12	HIS	-	EXPRESSION TAG	UNP P26948
C	13	HIS	-	EXPRESSION TAG	UNP P26948

- Molecule 4 is water.

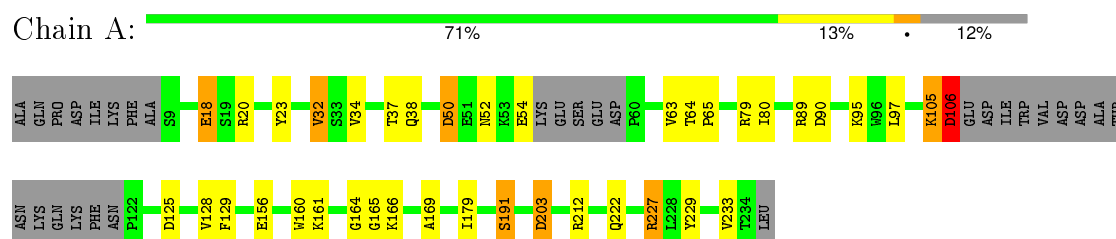
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	115	Total	O	0	0
			115	115		
4	C	70	Total	O	0	0
			70	70		

### 3 Residue-property plots [i](#)

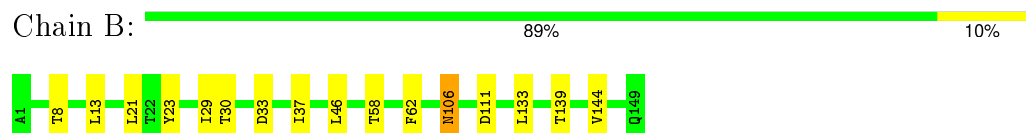
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

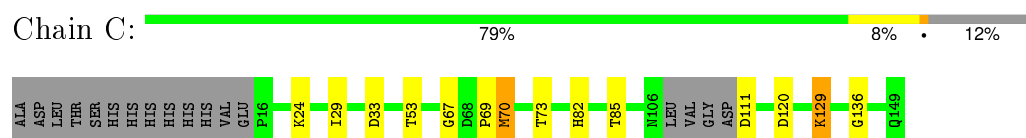
- Molecule 1: Chaperone protein Caf1M



- Molecule 2: F1 capsule antigen



- Molecule 3: F1 capsule antigen



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.82Å 69.62Å 45.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.71 – 1.99	Depositor
% Data completeness (in resolution range)	87.3 (87.71-1.99)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.166 , 0.216	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3982	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	1.24	7/1665 (0.4%)	1.16	13/2261 (0.6%)
2	B	1.19	2/1123 (0.2%)	1.01	0/1529
3	C	1.13	1/969 (0.1%)	1.12	5/1313 (0.4%)
All	All	1.20	10/3757 (0.3%)	1.10	18/5103 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	106	ASN	CB-CG	-8.08	1.32	1.51
1	A	32	VAL	CB-CG1	-7.53	1.37	1.52
1	A	165	GLY	N-CA	6.00	1.55	1.46
1	A	63	VAL	CB-CG2	-5.66	1.41	1.52
1	A	18	GLU	CG-CD	5.52	1.60	1.51
1	A	23	TYR	CZ-OH	5.45	1.47	1.37
1	A	164	GLY	N-CA	5.41	1.54	1.46
1	A	95	LYS	CD-CE	5.18	1.64	1.51
2	B	23	TYR	CE1-CZ	-5.07	1.31	1.38
3	C	67	GLY	C-O	-5.03	1.15	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASP	CB-CG-OD2	9.01	126.41	118.30
1	A	79	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	89	ARG	NE-CZ-NH2	-8.10	116.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	111	ASP	CB-CG-OD2	7.28	124.85	118.30
1	A	50[A]	ASP	CB-CG-OD2	7.16	124.74	118.30
1	A	50[B]	ASP	CB-CG-OD2	7.16	124.74	118.30
3	C	70	MET	CG-SD-CE	6.40	110.44	100.20
1	A	89	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	90	ASP	CB-CG-OD2	5.96	123.66	118.30
3	C	120	ASP	CB-CG-OD2	5.89	123.60	118.30
3	C	129	LYS	CD-CE-NZ	5.75	124.91	111.70
3	C	33	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	64	THR	OG1-CB-CG2	-5.47	97.42	110.00
1	A	37	THR	OG1-CB-CG2	-5.25	97.93	110.00
1	A	125	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	106	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	54	GLU	N-CA-C	5.07	124.68	111.00
1	A	161	LYS	CB-CA-C	-5.04	100.33	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	LYS	Peptide

## 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	1627	0	1615	15	0
2	B	1109	0	1083	9	0
3	C	956	0	930	7	0
4	A	105	0	0	2	0
4	B	115	0	0	1	0
4	C	70	0	0	1	0
All	All	3982	0	3628	27	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 (27) 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)
2:B:13:LEU:HD22	3:C:29:ILE:HB	1.70	0.73
1:A:212:ARG:NH2	1:A:233:VAL:O	2.31	0.63
1:A:160:TRP:CZ3	1:A:169:ALA:HB2	2.34	0.62
3:C:82:HIS:ND1	4:C:197:HOH:O	2.33	0.55
1:A:50[A]:ASP:OD2	1:A:52:ASN:ND2	2.38	0.55
1:A:222:GLN:HE21	3:C:136:GLY:HA2	1.72	0.54
1:A:179:ILE:HG22	1:A:191:SER:HB3	1.93	0.51
2:B:58:THR:HG23	2:B:111:ASP:CG	2.31	0.51
1:A:156:GLU:HG3	1:A:229:TYR:CD2	2.49	0.47
1:A:105:LYS:O	1:A:106:ASP:HB2	2.14	0.47
3:C:73:THR:HG23	3:C:129:LYS:HE3	1.96	0.47
2:B:58:THR:HG23	2:B:111:ASP:OD1	2.14	0.47
2:B:62:PHE:CD2	2:B:144:VAL:HG22	2.50	0.46
3:C:73:THR:CG2	3:C:129:LYS:HE3	2.46	0.45
1:A:166:LYS:HE3	1:A:203:ASP:OD1	2.16	0.45
1:A:18:GLU:HG2	1:A:32:VAL:HG23	1.99	0.45
2:B:37:ILE:HG23	2:B:133:LEU:HD12	1.98	0.44
1:A:128:VAL:HG21	2:B:29:ILE:HD12	1.99	0.44
2:B:33:ASP:CA	4:B:229:HOH:O	2.65	0.44
1:A:80:ILE:HD11	1:A:97:LEU:HD22	1.99	0.43
1:A:50[A]:ASP:OD1	1:A:50[A]:ASP:C	2.57	0.43
2:B:21:LEU:HD11	2:B:46:LEU:HD22	2.01	0.43
3:C:69:PRO:O	3:C:70:MET:HB2	2.19	0.43
1:A:227[B]:ARG:NH1	4:A:306:HOH:O	2.53	0.42
3:C:85:THR:CG2	3:C:129:LYS:HE2	2.49	0.41
1:A:38:GLN:NE2	4:A:296:HOH:O	2.54	0.41
1:A:129:PHE:O	2:B:139:THR:HA	2.21	0.41

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	205/235 (87%)	199 (97%)	6 (3%)	0	100	100
2	B	151/149 (101%)	149 (99%)	2 (1%)	0	100	100
3	C	126/147 (86%)	124 (98%)	2 (2%)	0	100	100
All	All	482/531 (91%)	472 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	176/204 (86%)	167 (95%)	9 (5%)	29	23
2	B	122/122 (100%)	118 (97%)	4 (3%)	45	43
3	C	105/122 (86%)	103 (98%)	2 (2%)	65	67
All	All	403/448 (90%)	388 (96%)	15 (4%)	51	38

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	34[A]	VAL
1	A	34[B]	VAL
1	A	34[C]	VAL
1	A	65	PRO
1	A	106	ASP
1	A	191	SER
1	A	227[A]	ARG
1	A	227[B]	ARG
2	B	8[A]	THR
2	B	8[B]	THR
2	B	30	THR
2	B	106	ASN
3	C	24	LYS
3	C	53	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	178	ASN
1	A	222	GLN
2	B	81	ASN

### 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](#)

There are no ligands in this entry.

### 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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.