Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:32 AM GMT

PDB ID	:	3ME0
Title	:	Structure of the E. coli chaperone PAPD in complex with the pilin domain of the PapGII adhesin
Authors	:	Ford, B.A.; Elam, J.S.; Dodson, K.W.; Pinkner, J.S.; Hultgren, S.J.
Deposited on	:	2010-03-31
Resolution	:	2.03 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

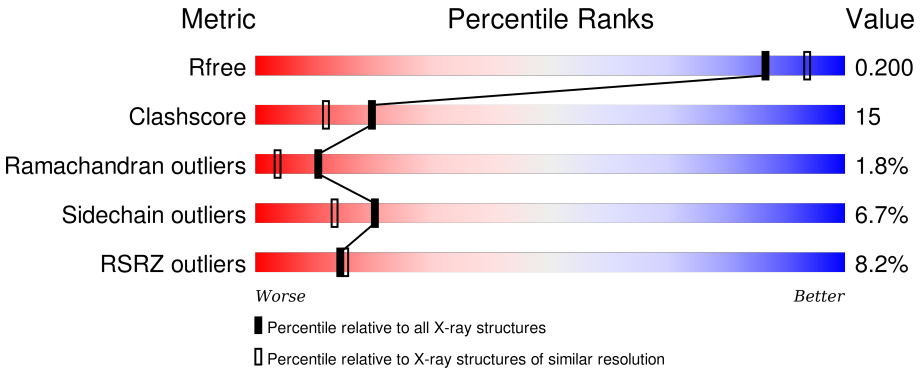
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.03 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))
R_{free}	91344	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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. 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	A	218	3%, 85%, 13%, ••
2	B	128	17%, 60%, 29%, 10%, •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3010 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 papD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	Se	5	1	0
			1716	1086	295	329	2	4			

- Molecule 2 is a protein called PapG protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	128	Total	C	N	O	S	0	2	0
			980	609	183	183	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	189	HIS	-	EXPRESSION TAG	UNP Q8FDY8
B	190	HIS	-	EXPRESSION TAG	UNP Q8FDY8
B	191	HIS	-	EXPRESSION TAG	UNP Q8FDY8
B	192	HIS	-	EXPRESSION TAG	UNP Q8FDY8
B	193	HIS	-	EXPRESSION TAG	UNP Q8FDY8
B	194	HIS	-	EXPRESSION TAG	UNP Q8FDY8

- Molecule 3 is water.

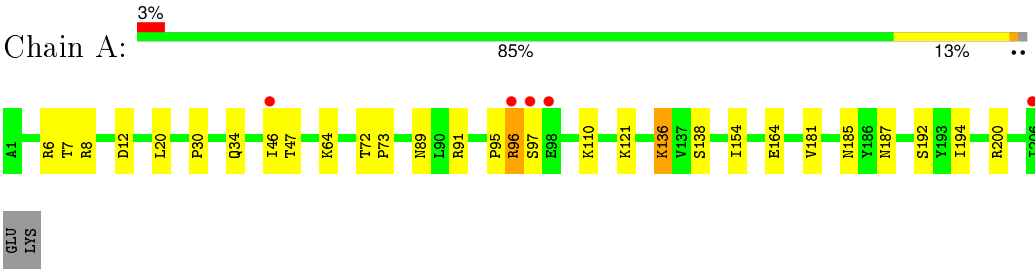
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	233	Total	O	0	0
			233	233		
3	B	81	Total	O	0	0
			81	81		

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.

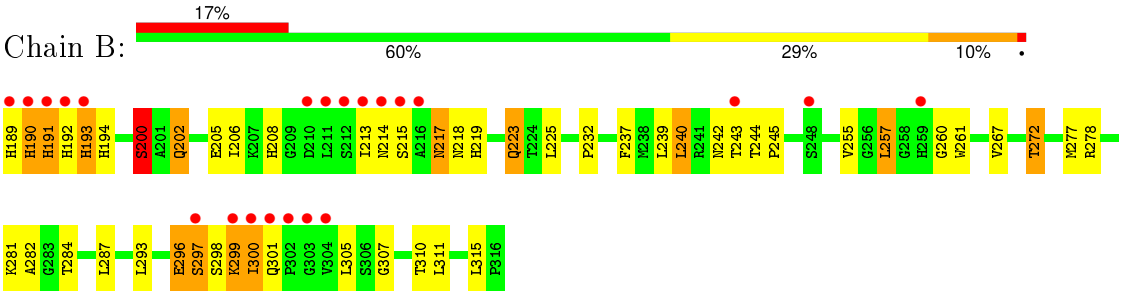
- Molecule 1: Chaperone protein papD

Chain A:



- Molecule 2: PapG protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	103.67Å 65.84Å 56.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.26 – 2.03 27.79 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.6 (28.26-2.03) 99.5 (27.79-2.03)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.190 0.192 , 0.200	Depositor DCC
R_{free} test set	1296 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 25464 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3010	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	1.04	1/1751 (0.1%)	0.56	0/2370
2	B	0.97	0/1014	0.58	0/1374
All	All	1.01	1/2765 (0.0%)	0.56	0/3744

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	ASN	CB-CG	5.33	1.63	1.51

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	1716	0	1733	31	0
2	B	980	0	945	54	0
3	A	233	0	0	2	0
3	B	81	0	0	4	0
All	All	3010	0	2678	80	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 15.

All (80) 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:96:ARG:CB	1:A:97:SER:HA	1.70	1.19
1:A:96:ARG:HB2	1:A:97:SER:HA	1.34	1.02
1:A:96:ARG:HB3	1:A:97:SER:HA	1.47	0.94
2:B:191:HIS:O	2:B:193:HIS:N	1.99	0.94
1:A:96:ARG:CB	1:A:97:SER:CA	2.48	0.92
2:B:300:ILE:HG22	2:B:301:GLN:N	1.82	0.92
1:A:95:PRO:HB2	1:A:96:ARG:HD3	1.52	0.91
1:A:96:ARG:HB3	1:A:97:SER:CA	2.03	0.89
2:B:300:ILE:CG2	2:B:301:GLN:H	1.88	0.86
2:B:300:ILE:CG2	2:B:301:GLN:N	2.41	0.83
1:A:216:LYS:HD3	1:A:216:LYS:C	2.00	0.81
1:A:136:LYS:HE3	1:A:185:ASN:HD22	1.45	0.79
2:B:244:THR:HG23	2:B:245:PRO:HD2	1.64	0.79
2:B:287:LEU:HD21	2:B:311:LEU:HD21	1.70	0.73
1:A:46:ILE:HD13	3:A:427:HOH:O	1.87	0.73
2:B:281:LYS:HG2	2:B:282:ALA:O	1.89	0.72
1:A:34:GLN:NE2	1:A:91:ARG:HE	1.89	0.71
2:B:300:ILE:O	2:B:301:GLN:HG3	1.91	0.71
2:B:217:ASN:O	2:B:293:LEU:O	2.11	0.69
2:B:200:SER:HB3	2:B:202:GLN:NE2	2.08	0.69
2:B:191:HIS:C	2:B:193:HIS:H	1.99	0.66
2:B:208:HIS:ND1	2:B:219:HIS:HD2	1.95	0.65
2:B:190:HIS:HD2	2:B:193:HIS:NE2	1.95	0.63
2:B:297:SER:N	2:B:300:ILE:HG12	2.14	0.63
2:B:300:ILE:HG22	2:B:301:GLN:H	1.47	0.63
2:B:260:GLY:HA3	2:B:300:ILE:HA	1.82	0.61
1:A:164:GLU:O	2:B:278:ARG:NH2	2.35	0.60
2:B:200:SER:HB3	2:B:202:GLN:HE22	1.64	0.60
2:B:191:HIS:C	2:B:193:HIS:N	2.56	0.59
1:A:96:ARG:HB3	1:A:97:SER:C	2.21	0.59
2:B:189:HIS:O	2:B:191:HIS:N	2.32	0.59
2:B:191:HIS:N	2:B:191:HIS:ND1	2.48	0.59
2:B:299:LYS:O	2:B:300:ILE:O	2.20	0.59
2:B:244:THR:CG2	2:B:245:PRO:HD2	2.32	0.57
2:B:214:ASN:O	2:B:215:SER:C	2.43	0.57
2:B:213:ILE:O	2:B:213:ILE:HD12	2.04	0.57
2:B:296:GLU:O	2:B:297:SER:HB2	2.06	0.56
1:A:12:ASP:OD1	1:A:121:LYS:HE2	2.05	0.56
1:A:154:ILE:HG21	1:A:194:ILE:HD11	1.88	0.54
1:A:97:SER:CB	2:B:205:GLU:OE2	2.57	0.54
2:B:300:ILE:HG23	2:B:301:GLN:H	1.70	0.53
2:B:272:THR:CG2	2:B:272:THR:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:LEU:HD12	2:B:307:GLY:HA3	1.92	0.52
2:B:261:TRP:CZ2	2:B:300:ILE:HD12	2.45	0.51
2:B:244:THR:HB	3:B:333:HOH:O	2.11	0.51
1:A:181:VAL:HG22	3:A:527:HOH:O	2.10	0.50
1:A:89:ASN:ND2	1:A:110:LYS:HG3	2.27	0.50
1:A:97:SER:HB2	2:B:205:GLU:OE2	2.11	0.50
1:A:89:ASN:HD21	1:A:110:LYS:HG3	1.77	0.50
2:B:237:PHE:CE1	2:B:277:MET:CE	2.96	0.49
1:A:95:PRO:HB2	1:A:96:ARG:CD	2.34	0.49
2:B:237:PHE:CE1	2:B:277:MET:HE2	2.48	0.48
2:B:244:THR:CB	3:B:333:HOH:O	2.61	0.48
2:B:202:GLN:NE2	3:B:475:HOH:O	2.47	0.48
2:B:189:HIS:O	2:B:189:HIS:CD2	2.67	0.47
1:A:34:GLN:HE21	1:A:91:ARG:HE	1.59	0.47
2:B:272:THR:O	2:B:272:THR:HG23	2.16	0.46
2:B:281:LYS:CG	2:B:282:ALA:N	2.78	0.46
2:B:242:ASN:ND2	3:B:352:HOH:O	2.46	0.45
1:A:200:ARG:HD2	2:B:232:PRO:HB2	1.97	0.45
2:B:296:GLU:O	2:B:297:SER:CB	2.63	0.45
2:B:243:THR:OG1	2:B:255:VAL:HG13	2.17	0.45
2:B:190:HIS:O	2:B:190:HIS:CG	2.70	0.45
1:A:7:THR:HB	2:B:315:LEU:HD23	2.00	0.44
1:A:96:ARG:HH11	1:A:96:ARG:HB2	1.81	0.44
2:B:225:LEU:HD21	2:B:287:LEU:HD23	1.99	0.44
1:A:30:PRO:O	1:A:95:PRO:HG3	2.18	0.43
2:B:261:TRP:CD1	2:B:305:LEU:HD21	2.54	0.42
1:A:72:THR:HB	1:A:73:PRO:HD2	2.01	0.42
2:B:206:ILE:HG12	2:B:223:GLN:HB2	2.00	0.42
2:B:217:ASN:HA	2:B:261:TRP:CZ3	2.54	0.42
1:A:89:ASN:HD21	1:A:110:LYS:NZ	2.18	0.42
2:B:239:LEU:HD11	2:B:267:VAL:HG13	2.02	0.42
1:A:6:ARG:NE	1:A:20:LEU:HD22	2.35	0.41
1:A:46:ILE:HD12	1:A:46:ILE:O	2.21	0.41
1:A:46:ILE:HG23	1:A:47:THR:HG23	2.02	0.41
2:B:240:LEU:HB2	2:B:310:THR:HB	2.02	0.41
1:A:154:ILE:HD11	1:A:192:SER:OG	2.22	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	215/218 (99%)	211 (98%)	4 (2%)	0	100 100
2	B	127/128 (99%)	111 (87%)	9 (7%)	7 (6%)	2 0
All	All	342/346 (99%)	322 (94%)	13 (4%)	7 (2%)	11 3

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	192[A]	HIS
2	B	192[B]	HIS
2	B	300	ILE
2	B	193	HIS
2	B	297	SER
2	B	190	HIS
2	B	200	SER

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	193/191 (101%)	186 (96%)	7 (4%)	42 38
2	B	109/107 (102%)	96 (88%)	13 (12%)	6 3
All	All	302/298 (101%)	282 (93%)	20 (7%)	20 14

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	64	LYS
1	A	96	ARG
1	A	136	LYS
1	A	138	SER
1	A	187	ASN
1	A	216	LYS
2	B	191	HIS
2	B	200	SER
2	B	202	GLN
2	B	217	ASN
2	B	218	ASN
2	B	223	GLN
2	B	240	LEU
2	B	257	LEU
2	B	272	THR
2	B	284	THR
2	B	296	GLU
2	B	298	SER
2	B	299	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	41	ASN
1	A	57	GLN
1	A	89	ASN
1	A	135	ASN
1	A	145	ASN
1	A	162	GLN
1	A	185	ASN
2	B	189	HIS
2	B	190	HIS
2	B	202	GLN
2	B	219	HIS
2	B	223	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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

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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	213/218 (97%)	0.05	6 (2%) 56 58	15, 27, 48, 78	0
2	B	128/128 (100%)	0.95	22 (17%) 2 2	18, 40, 83, 110	0
All	All	341/346 (98%)	0.39	28 (8%) 14 15	15, 31, 69, 110	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	189	HIS	8.2
2	B	191	HIS	8.1
2	B	213	ILE	7.9
2	B	215	SER	7.5
2	B	190	HIS	6.6
2	B	302	PRO	6.3
2	B	212	SER	6.3
2	B	192[A]	HIS	5.1
2	B	301	GLN	4.3
1	A	96	ARG	4.1
2	B	299	LYS	4.0
2	B	211	LEU	3.5
2	B	193	HIS	3.4
2	B	303	GLY	3.3
2	B	304	VAL	3.0
2	B	214	ASN	2.7
1	A	98	GLU	2.7
1	A	216	LYS	2.6
2	B	216	ALA	2.6
2	B	248	SER	2.5
2	B	243	THR	2.5
1	A	46	ILE	2.5
2	B	300	ILE	2.4
2	B	297	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	97	SER	2.2
2	B	210	ASP	2.2
2	B	259	HIS	2.1
1	A	206	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.