



wwPDB EM Map/Model Validation Report ⓘ

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PDB ID : 3J15
EMDB ID: : EMD-2009
Title : Model of ribosome-bound archaeal Pelota and ABCE1
Authors : Becker, T.; Franckenberg, S.; Wickles, S.; Shoemaker, C.J.; Anger, A.M.; Armache, J.-P.; Sieber, H.; Ungewickell, C.; Berninghausen, O.; Daberkow, I.; Karcher, A.; Thomm, M.; Hopfner, K.-P.; Green, R.; Beckmann, R.
Deposited on : 2011-12-12
Resolution : 6.60 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
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) : trunk27241

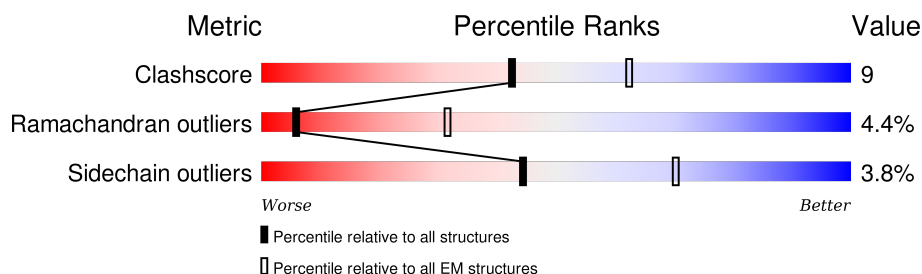
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	357	 68% 22% 9% .
2	B	593	 69% 25% 5%

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
3	ADP	B	601	-	-	X	-
3	ADP	B	602	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7660 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Protein pelota.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	357	2861	1818	503	533	7	0	0

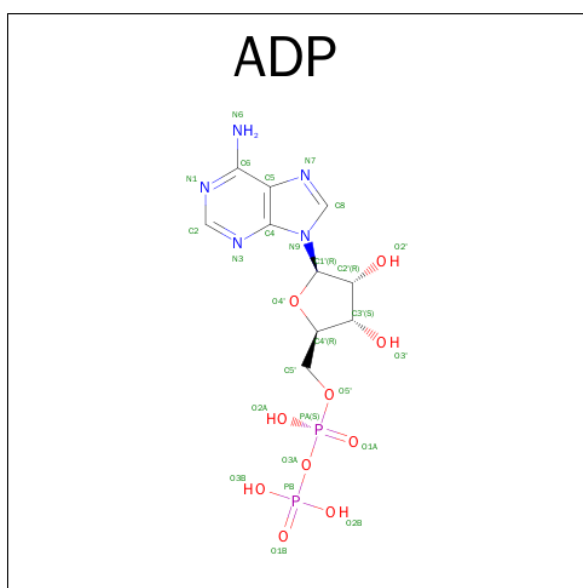
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	GLN	ENGINEERED MUTATION	UNP Q5JIB9

- Molecule 2 is a protein called ABC transporter ATP-binding protein.

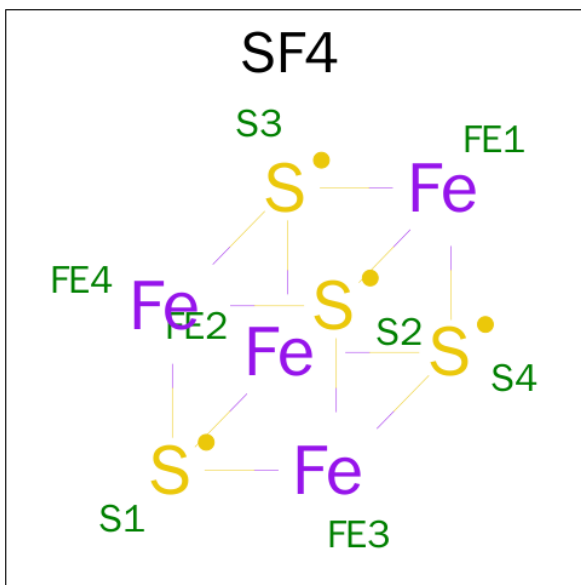
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	593	4729	3003	826	880	20	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			54	20	10	20	4	
3	B	1	Total	C	N	O	P	0
			54	20	10	20	4	

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

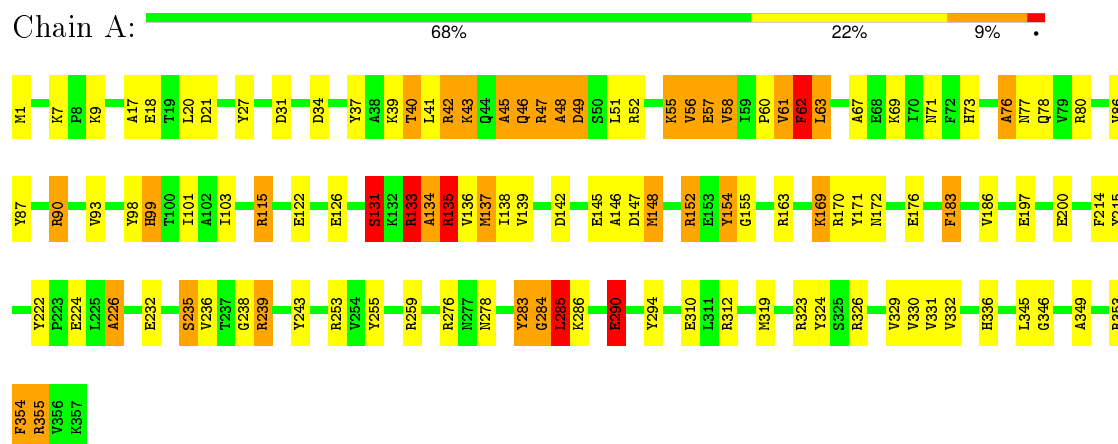


Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	Fe	S	0
			16	8	8	
4	B	1	Total	Fe	S	0
			16	8	8	

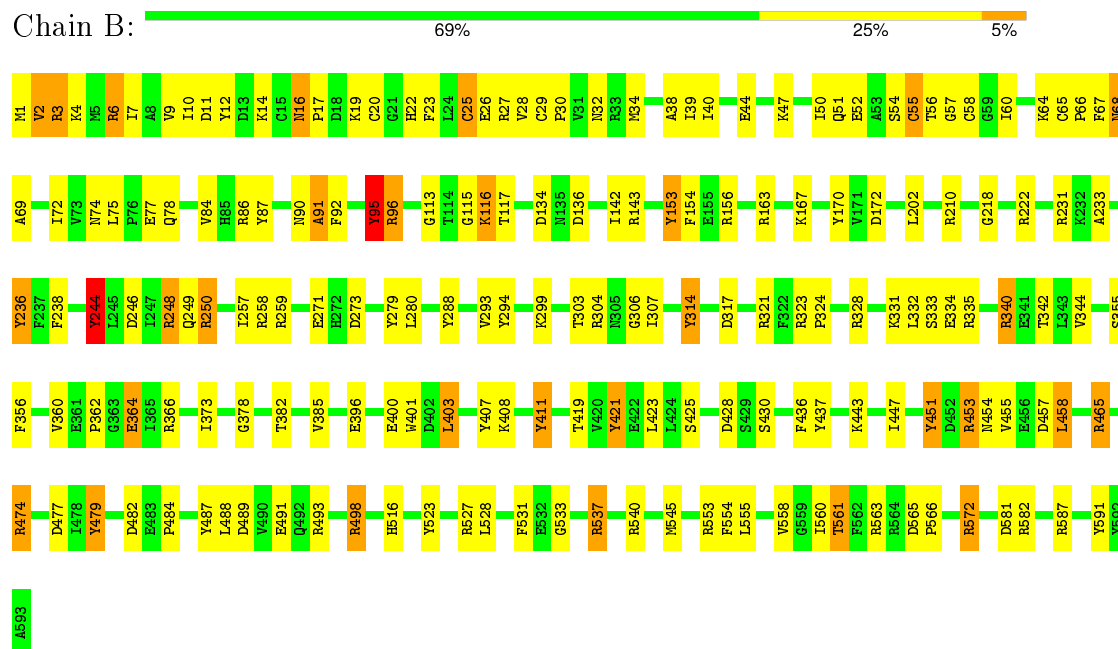
3 Residue-property plots

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. 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: Protein pelota



• Molecule 2: ABC transporter ATP-binding protein



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ADP

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.72	33/2903 (1.1%)	2.05	83/3904 (2.1%)
2	B	1.66	43/4815 (0.9%)	1.89	106/6499 (1.6%)
All	All	1.68	76/7718 (1.0%)	1.95	189/10403 (1.8%)

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	11
2	B	0	19
All	All	0	30

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	ARG	CD-NE	8.13	1.60	1.46
2	B	453	ARG	NE-CZ	7.92	1.43	1.33
1	A	154	TYR	CG-CD1	7.66	1.49	1.39
1	A	353	ARG	CZ-NH2	7.02	1.42	1.33
1	A	253	ARG	CZ-NH2	6.93	1.42	1.33

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ARG	NE-CZ-NH1	15.93	128.27	120.30
1	A	98	TYR	CB-CG-CD1	15.88	130.53	121.00
1	A	253	ARG	NE-CZ-NH1	15.54	128.07	120.30
1	A	239	ARG	NE-CZ-NH1	-15.17	112.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	453	ARG	NE-CZ-NH1	-14.70	112.95	120.30

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	ARG	Sidechain
1	A	147	ASP	Peptide
1	A	154	TYR	Sidechain
1	A	31	ASP	Peptide
1	A	73	HIS	Sidechain

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	2861	0	2947	46	0
2	B	4729	0	4777	96	0
3	B	54	0	24	27	0
4	B	16	0	0	1	0
All	All	7660	0	7748	134	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 9.

The worst 5 of 134 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:42:ARG:HB2	1:A:99:HIS:NE2	1.21	1.46
2:B:355:SER:OG	3:B:601:ADP:N3	1.65	1.26
1:A:40:THR:OG1	1:A:101:ILE:HD11	1.38	1.23
2:B:355:SER:OG	3:B:601:ADP:C2	1.92	1.21
1:A:42:ARG:HB2	1:A:99:HIS:CE1	1.76	1.20

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	355/357 (99%)	293 (82%)	36 (10%)	26 (7%)	1	21
2	B	591/593 (100%)	524 (89%)	51 (9%)	16 (3%)	6	45
All	All	946/950 (100%)	817 (86%)	87 (9%)	42 (4%)	6	33

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	55	LYS
1	A	60	PRO
1	A	61	VAL
1	A	63	LEU

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 PDB entries followed by that with respect to all EM entries.

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	305/305 (100%)	287 (94%)	18 (6%)	24	61
2	B	512/512 (100%)	499 (98%)	13 (2%)	55	81
All	All	817/817 (100%)	786 (96%)	31 (4%)	44	73

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	VAL

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Mol	Chain	Res	Type
1	A	331	VAL
2	B	447	ILE
1	A	283	TYR
2	B	2	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
2	B	249	GLN
2	B	74	ASN
1	A	78	GLN
2	B	16	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](#)

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	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	B	601	-	24,29,29	1.17	3 (12%)	23,45,45	0.89	1 (4%)
3	ADP	B	602	-	24,29,29	1.49	5 (20%)	23,45,45	1.02	1 (4%)
4	SF4	B	603	2	0,12,12	0.00	-	0,24,24	0.00	-
4	SF4	B	604	2	0,12,12	0.00	-	0,24,24	0.00	-

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
3	ADP	B	601	-	-	0/12/32/32	0/3/3/3
3	ADP	B	602	-	-	0/12/32/32	0/3/3/3
4	SF4	B	603	2	-	0/0/48/48	0/6/5/5
4	SF4	B	604	2	-	0/0/48/48	0/6/5/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ADP	C8-N7	-2.59	1.29	1.34
3	B	602	ADP	PB-O2B	-2.22	1.47	1.54
3	B	601	ADP	PB-O2B	-2.16	1.47	1.54
3	B	602	ADP	C2-N3	2.15	1.36	1.32
3	B	601	ADP	C4-N3	2.37	1.39	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	ADP	O2B-PB-O1B	2.08	117.42	110.63
3	B	602	ADP	O3B-PB-O2B	3.02	118.55	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	ADP	10	0
3	B	602	ADP	17	0
4	B	603	SF4	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.