wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:40 PM BST

PDB ID	:	3J1Z
EMDB ID:	:	EMD-5450
Title	:	Inward-Facing Conformation of the Zinc Transporter YiiP revealed by Cryo-electron Microscopy
Authors	:	Coudray, N.; Valvo, S.; Hu, M.; Lasala, R.; Kim, C.; Vink, M.; Zhou, M.; Provasi, D.; Filizola, M.; Tao, J.; Fang, J.; Penczek, P.A.; Ubarretxena-Belandia, I.; Stokes, D.L.; Transcontinental EM Initiative for Membrane Protein Structure (TEMIMPS)
Deposited on	:	2012-07-24
Resolution	:	13.00 Å(reported)
Based on PDB ID	:	3H90

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

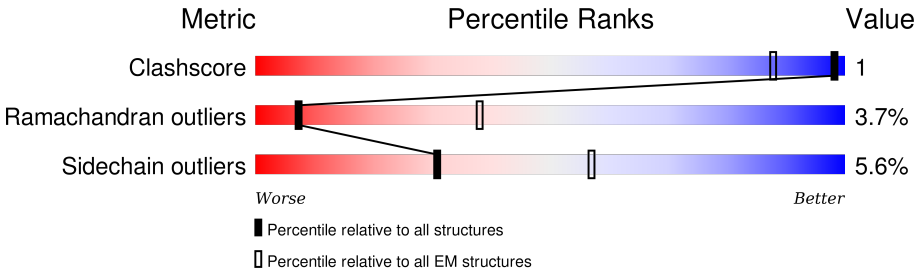
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 13.00 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 <=5%

Mol	Chain	Length	Quality of chain
1	P	306	84% 9%
1	Q	306	85% 10%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4586 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 Cation efflux family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	296	Total	C	N	O	S	0	0
			2293	1478	386	425	4		
1	Q	296	Total	C	N	O	S	0	0
			2293	1478	386	425	4		

There are 20 discrepancies between the modelled and reference sequences:

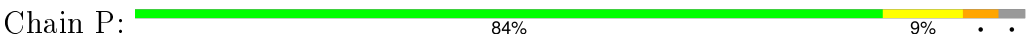
Chain	Residue	Modelled	Actual	Comment	Reference
P	297	HIS	-	EXPRESSION TAG	UNP Q8E919
P	298	HIS	-	EXPRESSION TAG	UNP Q8E919
P	299	HIS	-	EXPRESSION TAG	UNP Q8E919
P	300	HIS	-	EXPRESSION TAG	UNP Q8E919
P	301	HIS	-	EXPRESSION TAG	UNP Q8E919
P	302	HIS	-	EXPRESSION TAG	UNP Q8E919
P	303	HIS	-	EXPRESSION TAG	UNP Q8E919
P	304	HIS	-	EXPRESSION TAG	UNP Q8E919
P	305	HIS	-	EXPRESSION TAG	UNP Q8E919
P	306	HIS	-	EXPRESSION TAG	UNP Q8E919
Q	593	HIS	-	EXPRESSION TAG	UNP Q8E919
Q	594	HIS	-	EXPRESSION TAG	UNP Q8E919
Q	595	HIS	-	EXPRESSION TAG	UNP Q8E919
Q	596	HIS	-	EXPRESSION TAG	UNP Q8E919
Q	597	HIS	-	EXPRESSION TAG	UNP Q8E919
Q	598	HIS	-	EXPRESSION TAG	UNP Q8E919
Q	599	HIS	-	EXPRESSION TAG	UNP Q8E919
Q	600	HIS	-	EXPRESSION TAG	UNP Q8E919
Q	601	HIS	-	EXPRESSION TAG	UNP Q8E919
Q	602	HIS	-	EXPRESSION TAG	UNP Q8E919

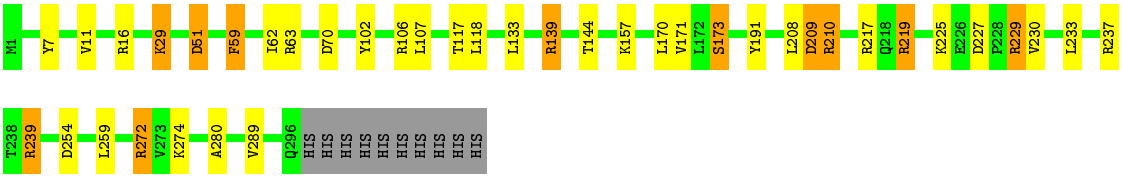
3 Residue-property plots (i)

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. 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: Cation efflux family protein

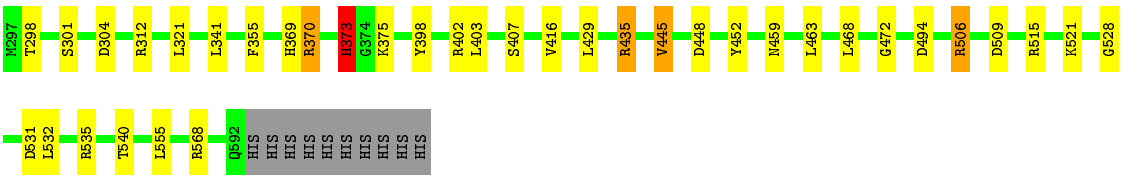
Chain P:





- Molecule 1: Cation efflux family protein

Chain Q:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Corrected throughout the reconstruction cycle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	10	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	50000	Depositor
Image detector	film	Depositor

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	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
1	P	0.70	0/2338	1.16	14/3187 (0.4%)
1	Q	0.69	0/2338	1.13	7/3187 (0.2%)
All	All	0.69	0/4676	1.14	21/6374 (0.3%)

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	P	0	12
1	Q	0	8
All	All	0	20

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	219	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	Q	402	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	Q	506	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	P	239	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	P	272	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	P	59	PHE	CB-CG-CD1	6.36	125.25	120.80
1	P	59	PHE	CB-CG-CD2	-6.13	116.51	120.80
1	Q	370	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	P	210	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	Q	398	TYR	CB-CG-CD2	-5.73	117.56	121.00
1	P	210	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	Q	370	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	P	209	ASP	CB-CG-OD2	5.44	123.19	118.30
1	P	229	ARG	NE-CZ-NH1	5.32	122.96	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	16	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	Q	515	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	P	272	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	P	219	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	Q	568	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	P	63	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	P	106	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	102	TYR	Sidechain
1	P	139	ARG	Sidechain
1	P	170	LEU	Peptide
1	P	173	SER	Peptide
1	P	191	TYR	Sidechain
1	P	210	ARG	Sidechain
1	P	217	ARG	Sidechain
1	P	219	ARG	Sidechain
1	P	237	ARG	Sidechain
1	P	239	ARG	Sidechain
1	P	272	ARG	Sidechain
1	P	280	ALA	Peptide
1	Q	298	THR	Peptide
1	Q	312	ARG	Sidechain
1	Q	373	HIS	Sidechain
1	Q	435	ARG	Sidechain
1	Q	452	TYR	Sidechain
1	Q	506	ARG	Sidechain
1	Q	531	ASP	Peptide
1	Q	535	ARG	Sidechain

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	P	2293	0	2326	4	0
1	Q	2293	0	2323	3	0
All	All	4586	0	4649	5	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 1.

All (5) 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:Q:373:HIS:CD2	1:Q:373:HIS:H	2.15	0.62
1:P:225:LYS:HA	1:P:230:VAL:HG21	1.85	0.58
1:P:208:LEU:HD23	1:Q:369:HIS:CD2	2.48	0.48
1:P:209:ASP:CG	1:Q:375:LYS:HZ2	2.21	0.43
1:P:29:LYS:HZ2	1:P:51:ASP:CG	2.24	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 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	P	294/306 (96%)	257 (87%)	27 (9%)	10 (3%)	5 40
1	Q	294/306 (96%)	258 (88%)	24 (8%)	12 (4%)	3 35
All	All	588/612 (96%)	515 (88%)	51 (9%)	22 (4%)	7 38

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	171	VAL
1	P	233	LEU
1	Q	301	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	304	ASP
1	Q	370	ARG
1	Q	407	SER
1	Q	509	ASP
1	Q	540	THR
1	P	51	ASP
1	P	144	THR
1	Q	373	HIS
1	Q	416	VAL
1	Q	445	VAL
1	P	7	TYR
1	P	11	VAL
1	P	70	ASP
1	P	117	THR
1	P	118	LEU
1	Q	463	LEU
1	Q	528	GLY
1	Q	472	GLY
1	P	289	VAL

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 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	P	242/252 (96%)	229 (95%)	13 (5%)	27	64
1	Q	242/252 (96%)	228 (94%)	14 (6%)	25	61
All	All	484/504 (96%)	457 (94%)	27 (6%)	31	62

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	29	LYS
1	P	59	PHE
1	P	62	ILE
1	P	107	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	133	LEU
1	P	139	ARG
1	P	157	LYS
1	P	173	SER
1	P	227	ASP
1	P	229	ARG
1	P	254	ASP
1	P	259	LEU
1	P	274	LYS
1	Q	321	LEU
1	Q	341	LEU
1	Q	355	PHE
1	Q	403	LEU
1	Q	429	LEU
1	Q	435	ARG
1	Q	445	VAL
1	Q	448	ASP
1	Q	459	ASN
1	Q	468	LEU
1	Q	494	ASP
1	Q	521	LYS
1	Q	532	LEU
1	Q	555	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	71	HIS
1	Q	490	GLN

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

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.