



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2017 – 02:19 PM EST

PDB ID : 5M8K
Title : Crystal structure of Eremococcus coleocola manganese transporter mutant E129Q
Authors : Manatschal, C.; Ehrnstorfer, I.A.; Arnold, F.M.; Laederach, J.; Dutzler, R.
Deposited on : 2016-10-29
Resolution : 3.60 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

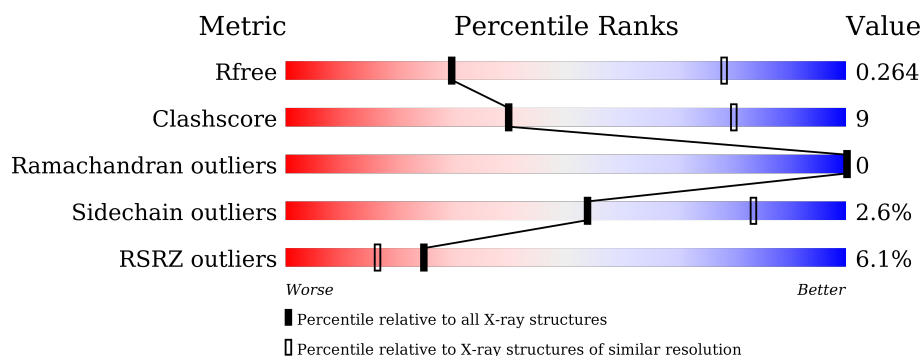
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	519	<div> <div>6%</div> <div>72%</div> <div>22%</div> <div>• 5%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3780 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 Divalent metal cation transporter MntH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3780	2475	625	663	17			

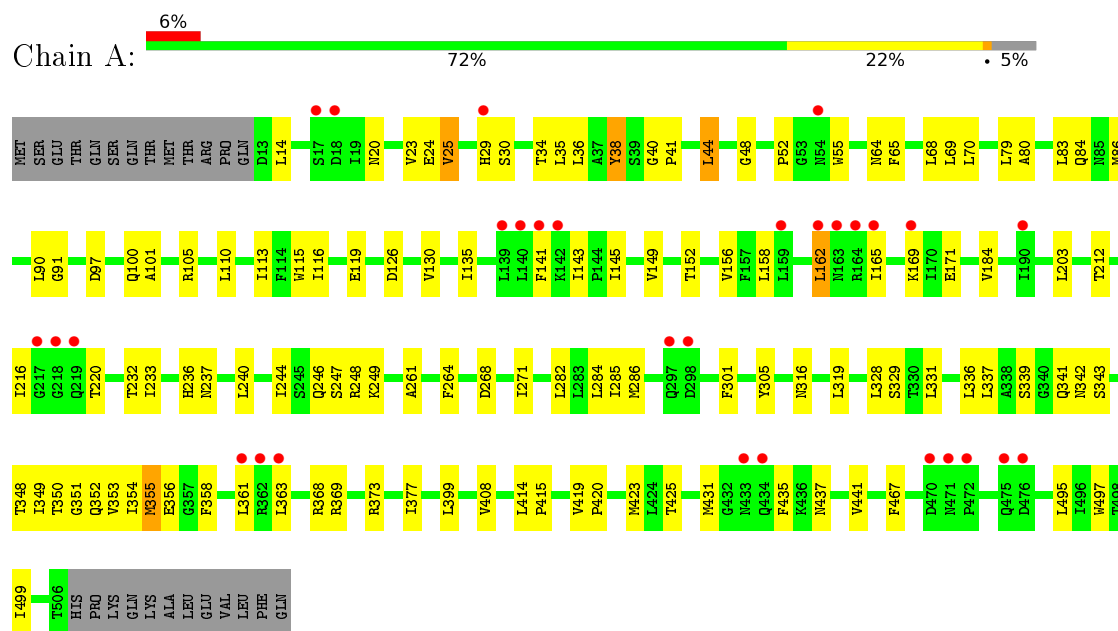
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP E4KPW4
A	1	SER	-	cloning artifact	UNP E4KPW4
A	129	GLN	GLU	engineered mutation	UNP E4KPW4
A	512	ALA	-	linker	UNP E4KPW4
A	513	LEU	-	linker	UNP E4KPW4
A	514	GLU	-	linker	UNP E4KPW4
A	515	VAL	-	linker	UNP E4KPW4
A	516	LEU	-	linker	UNP E4KPW4
A	517	PHE	-	linker	UNP E4KPW4
A	518	GLN	-	linker	UNP E4KPW4

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 ($\text{RSRZ} > 2$). 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: Divalent metal cation transporter MntH



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.26Å 81.77Å 96.50Å 90.00° 107.60° 90.00°	Depositor
Resolution (Å)	12.00 – 3.60 45.51 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (12.00-3.60) 91.5 (45.51-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.11 _2567: ???)	Depositor
R, R_{free}	0.221 , 0.265 0.229 , 0.264	Depositor DCC
R_{free} test set	634 reflections (5.71%)	DCC
Wilson B-factor (Å ²)	164.3	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 155.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	3780	wwPDB-VP
Average B, all atoms (Å ²)	213.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.24	0/3853	0.39	0/5253

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	A	3780	0	3982	68	0
All	All	3780	0	3982	68	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.

All (68) 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:14:LEU:HD13	1:A:20:ASN:HD22	1.51	0.75
1:A:158:LEU:O	1:A:162:LEU:HB2	1.95	0.65
1:A:319:LEU:HD12	1:A:328:LEU:HD21	1.77	0.65
1:A:348:THR:HG23	1:A:369:ARG:HH21	1.61	0.64
1:A:423:MET:HE1	1:A:499:ILE:HG23	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:SER:OG	1:A:248:ARG:NH2	2.31	0.64
1:A:156:VAL:HG22	1:A:369:ARG:HG3	1.82	0.61
1:A:343:SER:O	1:A:369:ARG:NH2	2.33	0.60
1:A:244:ILE:HD11	1:A:349:ILE:HG21	1.85	0.59
1:A:354:ILE:O	1:A:358:PHE:HB2	2.04	0.57
1:A:35:LEU:HA	1:A:38:TYR:CE1	2.39	0.57
1:A:282:LEU:HD23	1:A:285:ILE:HD11	1.87	0.55
1:A:126:ASP:OD1	1:A:373:ARG:NH1	2.40	0.55
1:A:119:GLU:OE1	1:A:368:ARG:NH2	2.37	0.54
1:A:316:ASN:HB3	1:A:319:LEU:HD23	1.89	0.54
1:A:24:GLU:HB3	1:A:249:LYS:HB3	1.90	0.53
1:A:351:GLY:O	1:A:355:MET:HB2	2.09	0.52
1:A:83:LEU:HD12	1:A:233:ILE:HG21	1.90	0.52
1:A:165:ILE:HG22	1:A:169:LYS:HB2	1.91	0.52
1:A:38:TYR:CZ	1:A:264:PHE:HB3	2.45	0.52
1:A:184:VAL:HG13	1:A:331:LEU:HB3	1.92	0.51
1:A:86:MET:HE3	1:A:425:THR:HG21	1.93	0.50
1:A:70:LEU:HB3	1:A:203:LEU:HD23	1.93	0.50
1:A:44:LEU:HD13	1:A:171:GLU:HG2	1.93	0.50
1:A:149:VAL:O	1:A:152:THR:OG1	2.25	0.50
1:A:282:LEU:O	1:A:286:MET:HB2	2.12	0.50
1:A:408:VAL:HG11	1:A:467:PHE:HZ	1.77	0.50
1:A:135:ILE:HG21	1:A:301:PHE:HB2	1.93	0.50
1:A:437:ASN:HB3	1:A:441:VAL:HG23	1.94	0.49
1:A:110:LEU:HD11	1:A:497:TRP:CD1	2.48	0.48
1:A:130:VAL:HG21	1:A:377:ILE:HG22	1.96	0.48
1:A:261:ALA:HA	1:A:264:PHE:CD2	2.48	0.47
1:A:301:PHE:HB3	1:A:336:LEU:HD11	1.96	0.47
1:A:65:PHE:HB3	1:A:68:LEU:HB3	1.96	0.47
1:A:34:THR:HG22	1:A:38:TYR:CE2	2.49	0.47
1:A:361:LEU:HG	1:A:363:LEU:HD13	1.97	0.47
1:A:352:GLN:O	1:A:356:GLU:HG2	2.14	0.46
1:A:64:ASN:ND2	1:A:216:ILE:O	2.49	0.46
1:A:305:TYR:CD2	1:A:329:SER:HB2	2.51	0.45
1:A:80:ALA:O	1:A:84:GLN:HB2	2.16	0.45
1:A:97:ASP:OD1	1:A:100:GLN:N	2.36	0.45
1:A:38:TYR:HA	1:A:248:ARG:HH11	1.82	0.45
1:A:23:VAL:HG12	1:A:25:VAL:HG22	1.99	0.45
1:A:337:LEU:O	1:A:341:GLN:HG2	2.16	0.45
1:A:52:PRO:HD3	1:A:339:SER:HB3	2.00	0.44
1:A:115:TRP:HE1	1:A:355:MET:HG3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:VAL:HB	1:A:420:PRO:HD3	1.99	0.44
1:A:52:PRO:HA	1:A:55:TRP:CG	2.53	0.43
1:A:212:THR:HA	1:A:220:THR:HB	2.01	0.43
1:A:48:GLY:HA2	1:A:342:ASN:ND2	2.34	0.43
1:A:79:LEU:HB2	1:A:232:THR:HG21	2.01	0.43
1:A:232:THR:HG22	1:A:233:ILE:HG23	2.01	0.42
1:A:349:ILE:O	1:A:353:VAL:HG23	2.19	0.42
1:A:236:HIS:HB2	1:A:350:THR:HG21	2.00	0.42
1:A:40:GLY:N	1:A:41:PRO:HD2	2.35	0.42
1:A:90:LEU:HG	1:A:431:MET:HE1	2.02	0.42
1:A:52:PRO:HA	1:A:55:TRP:CD1	2.55	0.42
1:A:113:ILE:HD13	1:A:116:ILE:HD11	2.03	0.41
1:A:237:ASN:HA	1:A:240:LEU:HB3	2.02	0.41
1:A:24:GLU:N	1:A:24:GLU:OE1	2.53	0.41
1:A:419:VAL:HG21	1:A:495:LEU:HD11	2.03	0.41
1:A:69:LEU:HB2	1:A:284:LEU:HD11	2.02	0.41
1:A:101:ALA:O	1:A:105:ARG:HG2	2.21	0.41
1:A:145:ILE:HD11	1:A:399:LEU:HD11	2.03	0.40
1:A:40:GLY:CA	1:A:171:GLU:HB3	2.51	0.40
1:A:414:LEU:HB3	1:A:415:PRO:HD3	2.03	0.40
1:A:141:PHE:HB2	1:A:143:ILE:HG13	2.03	0.40
1:A:91:GLY:O	1:A:246:GLN:HG2	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	492/519 (95%)	463 (94%)	29 (6%)	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	Percentiles
1	A	418/442 (95%)	407 (97%)	11 (3%)	54 83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	29	HIS
1	A	30	SER
1	A	36	LEU
1	A	38	TYR
1	A	44	LEU
1	A	162	LEU
1	A	268	ASP
1	A	271	ILE
1	A	355	MET
1	A	435	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	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 ⓘ

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, 95th 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	494/519 (95%)	-0.22	30 (6%) 25 16	139, 205, 294, 352	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	433	ASN	7.8
1	A	297	GLN	5.9
1	A	218	GLY	5.6
1	A	470	ASP	5.5
1	A	141	PHE	4.8
1	A	471	ASN	4.8
1	A	217	GLY	3.8
1	A	18	ASP	3.6
1	A	298	ASP	3.6
1	A	219	GLN	3.6
1	A	165	ILE	3.5
1	A	164	ARG	3.5
1	A	140	LEU	3.4
1	A	475	GLN	3.1
1	A	363	LEU	3.0
1	A	434	GLN	2.9
1	A	159	LEU	2.6
1	A	162	LEU	2.6
1	A	29	HIS	2.4
1	A	163	ASN	2.4
1	A	472	PRO	2.3
1	A	17	SER	2.3
1	A	169	LYS	2.3
1	A	361	LEU	2.2
1	A	476	ASP	2.2
1	A	190	ILE	2.2
1	A	142	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	362	ARG	2.1
1	A	139	LEU	2.1
1	A	54	ASN	2.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.