



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2ZY9 / pdb_00002zy9
Title : Improved crystal structure of magnesium transporter MgtE
Authors : Nureki, O.; Ishitani, R.; Hattori, M.
Deposited on : 2009-01-19
Resolution : 2.94 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

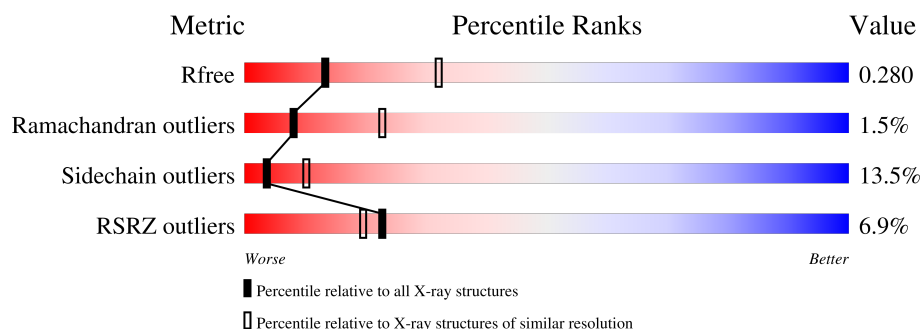
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	180053	1159 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	473	7% 80%10%10%
1	B	473	6% 78%12%9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6468 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 Mg²⁺ transporter MgtE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3242	2105	525	605	7			
1	B	429	Total	C	N	O	S	0	0	0
			3213	2094	507	605	7			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q5SMG8
A	-21	GLY	-	expression tag	UNP Q5SMG8
A	-20	SER	-	expression tag	UNP Q5SMG8
A	-19	SER	-	expression tag	UNP Q5SMG8
A	-18	HIS	-	expression tag	UNP Q5SMG8
A	-17	HIS	-	expression tag	UNP Q5SMG8
A	-16	HIS	-	expression tag	UNP Q5SMG8
A	-15	HIS	-	expression tag	UNP Q5SMG8
A	-14	HIS	-	expression tag	UNP Q5SMG8
A	-13	HIS	-	expression tag	UNP Q5SMG8
A	-12	SER	-	expression tag	UNP Q5SMG8
A	-11	SER	-	expression tag	UNP Q5SMG8
A	-10	GLY	-	expression tag	UNP Q5SMG8
A	-9	LEU	-	expression tag	UNP Q5SMG8
A	-8	GLY	-	expression tag	UNP Q5SMG8
A	-7	VAL	-	expression tag	UNP Q5SMG8
A	-6	LEU	-	expression tag	UNP Q5SMG8
A	-5	PRO	-	expression tag	UNP Q5SMG8
A	-4	GLY	-	expression tag	UNP Q5SMG8
A	-3	GLY	-	expression tag	UNP Q5SMG8
A	-2	PRO	-	expression tag	UNP Q5SMG8
A	-1	LEU	-	expression tag	UNP Q5SMG8
A	0	HIS	-	expression tag	UNP Q5SMG8
B	-22	MET	-	expression tag	UNP Q5SMG8
B	-21	GLY	-	expression tag	UNP Q5SMG8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	expression tag	UNP Q5SMG8
B	-19	SER	-	expression tag	UNP Q5SMG8
B	-18	HIS	-	expression tag	UNP Q5SMG8
B	-17	HIS	-	expression tag	UNP Q5SMG8
B	-16	HIS	-	expression tag	UNP Q5SMG8
B	-15	HIS	-	expression tag	UNP Q5SMG8
B	-14	HIS	-	expression tag	UNP Q5SMG8
B	-13	HIS	-	expression tag	UNP Q5SMG8
B	-12	SER	-	expression tag	UNP Q5SMG8
B	-11	SER	-	expression tag	UNP Q5SMG8
B	-10	GLY	-	expression tag	UNP Q5SMG8
B	-9	LEU	-	expression tag	UNP Q5SMG8
B	-8	GLY	-	expression tag	UNP Q5SMG8
B	-7	VAL	-	expression tag	UNP Q5SMG8
B	-6	LEU	-	expression tag	UNP Q5SMG8
B	-5	PRO	-	expression tag	UNP Q5SMG8
B	-4	GLY	-	expression tag	UNP Q5SMG8
B	-3	GLY	-	expression tag	UNP Q5SMG8
B	-2	PRO	-	expression tag	UNP Q5SMG8
B	-1	LEU	-	expression tag	UNP Q5SMG8
B	0	HIS	-	expression tag	UNP Q5SMG8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total Mg 7 7	0	0
2	B	6	Total Mg 6 6	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.36Å 76.53Å 160.04Å 90.00° 102.17° 90.00°	Depositor
Resolution (Å)	26.71 – 2.94 26.71 – 2.94	Depositor EDS
% Data completeness (in resolution range)	95.0 (26.71-2.94) 95.3 (26.71-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.255 , 0.295 (Not available) , 0.280	Depositor DCC
R_{free} test set	1685 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6468	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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

5.1 Standard geometry

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

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	0.35	0/3302	0.81	8/4527 (0.2%)
1	B	0.34	0/3273	0.82	3/4498 (0.1%)
All	All	0.35	0/6575	0.81	11/9025 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASN	CA-C-N	8.66	128.66	119.05
1	A	203	ASN	C-N-CA	8.66	128.66	119.05
1	A	76	LEU	CA-C-N	7.03	124.79	119.66
1	A	76	LEU	C-N-CA	7.03	124.79	119.66
1	B	295	THR	N-CA-C	-6.55	105.83	113.88
1	B	76	LEU	CA-C-N	5.74	123.85	119.66
1	B	76	LEU	C-N-CA	5.74	123.85	119.66
1	A	77	PRO	CA-C-N	5.50	125.17	119.56
1	A	77	PRO	C-N-CA	5.50	125.17	119.56
1	A	104	ASP	CA-C-N	5.14	124.45	118.85
1	A	104	ASP	C-N-CA	5.14	124.45	118.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	425/473 (90%)	372 (88%)	48 (11%)	5 (1%)	10	27
1	B	427/473 (90%)	367 (86%)	52 (12%)	8 (2%)	6	17
All	All	852/946 (90%)	739 (87%)	100 (12%)	13 (2%)	8	23

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	269	PRO
1	A	103	GLU
1	A	395	VAL
1	A	402	ASN
1	A	213	THR
1	B	64	LEU
1	B	87	GLU
1	B	254	ALA
1	A	422	VAL
1	B	422	VAL
1	B	278	PRO
1	B	291	ILE
1	B	117	PRO

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	339/400 (85%)	298 (88%)	41 (12%)	5	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	333/400 (83%)	283 (85%)	50 (15%)	3	8
All	All	672/800 (84%)	581 (86%)	91 (14%)	4	10

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	81	LEU
1	A	90	LEU
1	A	111	LEU
1	A	128	ARG
1	A	132	ASP
1	A	141	GLU
1	A	168	ILE
1	A	174	VAL
1	A	176	GLU
1	A	206	VAL
1	A	213	THR
1	A	217	GLU
1	A	222	MET
1	A	228	THR
1	A	249	LEU
1	A	255	GLU
1	A	292	LEU
1	A	293	ILE
1	A	299	THR
1	A	300	SER
1	A	302	ILE
1	A	310	LEU
1	A	313	VAL
1	A	314	THR
1	A	330	THR
1	A	336	THR
1	A	337	LEU
1	A	340	ARG
1	A	357	LEU
1	A	364	LEU
1	A	389	VAL
1	A	396	LEU
1	A	398	VAL
1	A	408	LEU
1	A	421	LEU

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Mol	Chain	Res	Type
1	A	423	SER
1	A	427	VAL
1	A	429	THR
1	A	430	LEU
1	A	447	LEU
1	B	28	ILE
1	B	39	GLU
1	B	51	LEU
1	B	60	VAL
1	B	61	LEU
1	B	65	SER
1	B	75	THR
1	B	76	LEU
1	B	80	ARG
1	B	81	LEU
1	B	90	LEU
1	B	97	LEU
1	B	100	VAL
1	B	115	LEU
1	B	119	THR
1	B	123	VAL
1	B	137	LEU
1	B	160	ARG
1	B	171	ILE
1	B	174	VAL
1	B	196	THR
1	B	198	VAL
1	B	201	ILE
1	B	228	THR
1	B	233	VAL
1	B	235	GLU
1	B	244	THR
1	B	248	VAL
1	B	252	LEU
1	B	257	THR
1	B	258	GLU
1	B	260	ILE
1	B	279	VAL
1	B	286	VAL
1	B	289	LEU
1	B	291	ILE
1	B	292	LEU

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Mol	Chain	Res	Type
1	B	294	LEU
1	B	300	SER
1	B	302	ILE
1	B	303	LEU
1	B	322	VAL
1	B	330	THR
1	B	365	LEU
1	B	387	LEU
1	B	389	VAL
1	B	411	LEU
1	B	421	LEU
1	B	430	LEU
1	B	446	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	109	GLN
1	A	215	GLN
1	A	383	HIS
1	B	44	HIS
1	B	215	GLN
1	B	329	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	427/473 (90%)	0.60	31 (7%)	21 18	68, 106, 150, 184	0
1	B	429/473 (90%)	0.58	28 (6%)	25 21	80, 123, 175, 235	0
All	All	856/946 (90%)	0.59	59 (6%)	23 19	68, 115, 164, 235	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	PRO	6.6
1	A	385	LEU	6.5
1	A	325	GLY	6.2
1	B	24	VAL	5.3
1	B	385	LEU	5.0
1	A	328	GLY	4.9
1	B	380	TRP	4.5
1	A	326	THR	3.7
1	B	127	ALA	3.6
1	A	353	ARG	3.5
1	B	114	LEU	3.4
1	A	96	ALA	3.4
1	B	386	LEU	3.3
1	A	88	LEU	3.3
1	A	340	ARG	3.3
1	B	148	GLY	3.3
1	A	343	ALA	3.2
1	A	318	PHE	3.1
1	B	242	ILE	3.1
1	B	128	ARG	3.1
1	A	148	GLY	2.9
1	A	382	GLY	2.9
1	B	323	LEU	2.8
1	A	449	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	271	LEU	2.8
1	A	79	TRP	2.7
1	A	323	LEU	2.7
1	A	214	ASP	2.7
1	B	312	ALA	2.7
1	A	62	SER	2.6
1	B	310	LEU	2.5
1	B	177	LYS	2.5
1	B	22	ARG	2.5
1	B	44	HIS	2.5
1	A	448	GLU	2.5
1	B	446	LEU	2.4
1	B	199	ALA	2.4
1	B	343	ALA	2.4
1	A	166	GLU	2.4
1	B	202	MET	2.4
1	B	40	LEU	2.4
1	A	299	THR	2.3
1	A	305	GLY	2.3
1	B	143	VAL	2.3
1	B	265	ALA	2.3
1	A	216	GLU	2.2
1	A	49	LEU	2.2
1	B	20	ALA	2.2
1	A	103	GLU	2.2
1	A	114	LEU	2.1
1	A	63	HIS	2.1
1	A	43	GLU	2.1
1	A	54	LYS	2.1
1	B	320	VAL	2.1
1	B	387	LEU	2.1
1	A	147	GLU	2.1
1	B	116	ASP	2.1
1	B	267	ASP	2.1
1	B	113	ASP	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	B	451	1/1	0.83	0.17	90,90,90,90	0
2	MG	A	453	1/1	0.85	0.24	75,75,75,75	0
2	MG	B	453	1/1	0.85	0.26	74,74,74,74	0
2	MG	A	456	1/1	0.86	0.26	79,79,79,79	0
2	MG	B	454	1/1	0.88	0.36	81,81,81,81	0
2	MG	A	457	1/1	0.90	0.20	75,75,75,75	0
2	MG	B	456	1/1	0.90	0.35	98,98,98,98	0
2	MG	A	455	1/1	0.95	0.28	62,62,62,62	0
2	MG	A	451	1/1	0.96	0.53	72,72,72,72	0
2	MG	B	452	1/1	0.97	0.24	78,78,78,78	0
2	MG	A	454	1/1	0.97	0.23	60,60,60,60	0
2	MG	B	455	1/1	0.98	0.16	61,61,61,61	0
2	MG	A	452	1/1	0.98	0.17	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.