



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:32 PM UTC

PDB ID : 7NDY / pdb_00007ndy
Title : Di-phosphorylated Barrier-to-Autointegration Factor (BAF) in complex with LEM domain of Emerin
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Deposited on : 2021-02-02
Resolution : 1.44 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

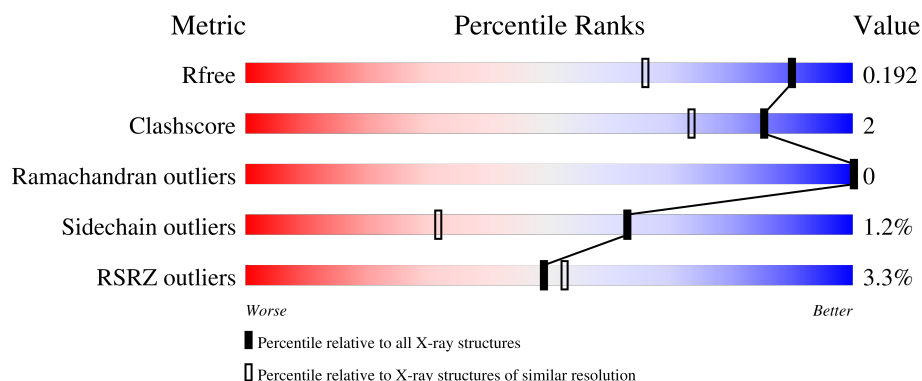
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.44 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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 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	89	0% 89% 9% ..
1	B	89	2% 93% 6% .
2	G	187	2% 21% 78% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2008 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 Barrier-to-autointegration factor, N-terminally processed.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	88	Total	C	N	O	P	S	0	4	0
			723	457	124	139	2	1			
1	B	88	Total	C	N	O	P	S	0	2	0
			710	448	120	139	2	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O75531
A	67	ALA	CYS	conflict	UNP O75531
A	77	ALA	CYS	conflict	UNP O75531
A	80	ALA	CYS	conflict	UNP O75531
A	85	ALA	CYS	conflict	UNP O75531
B	1	GLY	-	expression tag	UNP O75531
B	67	ALA	CYS	conflict	UNP O75531
B	77	ALA	CYS	conflict	UNP O75531
B	80	ALA	CYS	conflict	UNP O75531
B	85	ALA	CYS	conflict	UNP O75531

- Molecule 2 is a protein called Emerin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	42	Total	C	N	O	0	1	0
			352	223	61	68			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	GLY	-	expression tag	UNP P50402

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	B	85	Total	O	0	0
			85	85		
4	G	42	Total	O	0	0
			42	42		

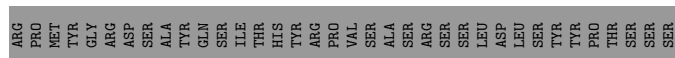
i

- Molecule 1: Barrier-to-autointegration factor, N-terminally processed



-

- GLY
 ASP
 N3
 Y4
 A5
 D6
 L7
 L15
 Y19
 Q44
 ARG
 ARG
 ARG
 LEU
 SER
 PRO
 PRO
 SER
 SER
 SER
 ALA
 ALA
 SER
 SER
 TYR
 TYR
 PHE
 SER
 ASP
 LEU
 ASN
 SER
 THR
 THR
 ARG
 GLY
 ASP
 ASP
 MET
 TYR
 ASP
 PRO
 PRO
 LYS
 LYS
 GLU
 ASP
 ASP
 LEU
 LEU
 TYR
 GLN
 SER
 SER
 LYS
 GLY
 TYR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	33.05Å 40.63Å 43.22Å 69.51° 69.68° 85.03°	Depositor
Resolution (Å)	38.03 – 1.44 38.03 – 1.44	Depositor EDS
% Data completeness (in resolution range)	57.2 (38.03-1.44) 57.2 (38.03-1.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.44Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.181 , 0.225 0.190 , 0.192	Depositor DCC
R_{free} test set	1022 reflections (2.86%)	wwPDB-VP
Wilson B-factor (Å ²)	12.4	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2008	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.15% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, TPO, EPE

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	0.68	0/726	0.95	0/968
1	B	0.75	0/707	0.93	1/944 (0.1%)
2	G	0.67	0/362	0.92	0/490
All	All	0.71	0/1795	0.94	1/2402 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	PHE	CA-CB-CG	6.07	119.87	113.80

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	723	0	721	5	0
1	B	710	0	697	2	0
2	G	352	0	345	1	0
3	B	15	0	17	0	0
4	A	81	0	0	1	0
4	B	85	0	0	1	0
4	G	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2008	0	1780	8	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 2.

All (8) 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:64[A]:LYS:HZ3	1:A:70:ASN:C	2.15	0.55
1:A:64[B]:LYS:HE3	1:A:71:ALA:HA	1.92	0.51
1:B:54:LYS:NZ	4:B:203:HOH:O	2.41	0.46
4:A:127:HOH:O	1:B:53:LYS:HD2	2.16	0.46
2:G:15:LEU:HD22	2:G:19:TYR:CE2	2.52	0.44
1:A:62:TRP:CE2	1:A:66:THR:HG21	2.56	0.41
1:A:30:LEU:HD11	1:A:69:ALA:HA	2.03	0.40
1:A:64[A]:LYS:NZ	1:A:70:ASN:C	2.80	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	88/89 (99%)	87 (99%)	1 (1%)	0	100	100
1	B	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
2	G	41/187 (22%)	41 (100%)	0	0	100	100
All	All	215/365 (59%)	212 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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 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	71/67 (106%)	70 (99%)	1 (1%)	59	26
1	B	69/67 (103%)	69 (100%)	0	100	100
2	G	39/168 (23%)	38 (97%)	1 (3%)	40	9
All	All	179/302 (59%)	177 (99%)	2 (1%)	63	35

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	THR
2	G	7	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	TPO	B	3	1	8,10,11	0.67	0	10,14,16	1.93	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	A	4	1	8,9,10	0.92	0	7,12,14	1.50	1 (14%)
1	SEP	B	4	1	8,9,10	0.61	0	7,12,14	2.31	1 (14%)
1	TPO	A	3	1	8,10,11	1.08	1 (12%)	10,14,16	1.79	3 (30%)

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
1	TPO	B	3	1	-	1/9/11/13	-
1	SEP	A	4	1	-	2/6/8/10	-
1	SEP	B	4	1	-	0/6/8/10	-
1	TPO	A	3	1	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	TPO	CG2-CB	2.26	1.57	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	SEP	OG-CB-CA	-5.72	102.58	108.14
1	B	3	TPO	CG2-CB-CA	-3.65	106.15	113.26
1	B	3	TPO	P-OG1-CB	-3.52	113.76	123.33
1	A	3	TPO	CG2-CB-CA	-3.45	106.53	113.26
1	A	4	SEP	OG-CB-CA	-3.24	104.99	108.14
1	A	3	TPO	P-OG1-CB	-2.77	115.80	123.33
1	B	3	TPO	O-C-CA	-2.47	118.41	124.77
1	A	3	TPO	O-C-CA	-2.14	119.27	124.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	4	SEP	CB-OG-P-O3P
1	A	4	SEP	CB-OG-P-O2P
1	A	3	TPO	O-C-CA-CB
1	B	3	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	EPE	B	101	-	15,15,15	1.39	1 (6%)	19,20,20	0.40	0

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	EPE	B	101	-	-	2/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	101	EPE	C10-S	-5.22	1.70	1.77

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	101	EPE	C9-C10-S-O2S
3	B	101	EPE	C9-C10-S-O3S

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	86/89 (96%)	0.14	1 (1%) 76 80	7, 12, 22, 26	4 (4%)
1	B	86/89 (96%)	0.02	2 (2%) 61 65	7, 12, 19, 23	2 (2%)
2	G	42/187 (22%)	0.47	4 (9%) 14 15	8, 17, 34, 42	1 (2%)
All	All	214/365 (58%)	0.15	7 (3%) 49 52	7, 13, 23, 42	7 (3%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	6	ASP	3.1
2	G	4	TYR	2.9
1	B	40	ASP	2.4
2	G	3	ASN	2.4
1	B	2	THR	2.3
2	G	7	LEU	2.3
1	A	2	THR	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	A	4	10/11	0.89	0.11	17,22,53,55	0
1	TPO	A	3	11/12	0.91	0.10	18,22,29,31	0
1	SEP	B	4	10/11	0.95	0.06	12,13,19,19	0
1	TPO	B	3	11/12	0.96	0.06	14,19,29,30	0

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($\text{\AA}^2$)	Q<0.9
3	EPE	B	101	15/15	0.94	0.09	19,20,21,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.