

wwPDB EM Validation Summary Report (i)

Oct 18, 2022 – 09:40 pm BST

PDB ID : 7015

EMDB ID : EMD-12690

Title: ABC transporter NosDFY, nucleotide-free in lipid nanodisc, R-domain 2

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Deposited on : 2021-03-28 Resolution : Not provided

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43

MolProbity : 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

MapQ : FAILED

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

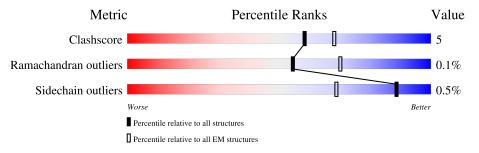
Validation Pipeline (wwPDB-VP) : 2.31.2

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 unknown.

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 $(\# ext{Entries})$	${ m EM~structures} \ (\#{ m Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

Mol	Chain	Length	Quality of chain				
1	A	436	71% 21%	8%			
2	В	308	89%	11%			
2	С	308	89%	11%			
3	D	276	87%	10% •			
3	Е	276	85%	• 10%			



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11787 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 Probable ABC transporter binding protein NosD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	402	Total 3140	C 1950	N 566	O 613	S 11	0	0

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

Mol	Chain	Residues	${f Atoms}$				AltConf	Trace	
2	В	307	Total 2367	C 1478	N 442	0	\sim	0	0
2	С	307	Total 2367	C 1478				0	0

• Molecule 3 is a protein called Probable ABC transporter permease protein NosY.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	267	Total	С	N	О	S	0	0
9	D	201	2015	1355	319	334	7		0
9	E	248	Total	С	N	О	S	0	0
3	E	240	1896	1284	300	306	6	0	U

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atom	ıs	AltConf
4	A	1	Total 1	Mg 1	0

• Molecule 5 is water.

\mathbf{Mol}	Chain	Residues	Atoms	AltConf
5	A	1	Total O 1 1	0



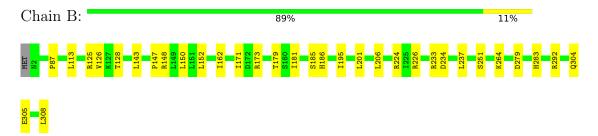
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

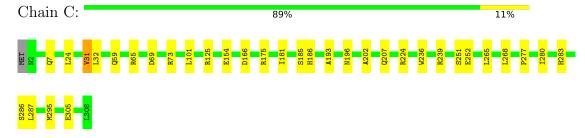
• Molecule 1: Probable ABC transporter binding protein NosD



• Molecule 2: Probable ABC transporter ATP-binding protein NosF

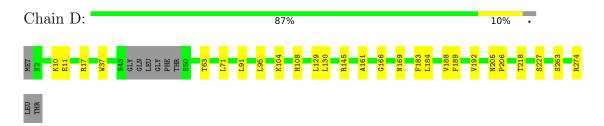


• Molecule 2: Probable ABC transporter ATP-binding protein NosF

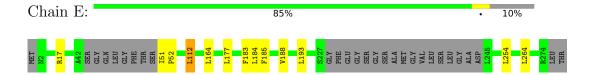


• Molecule 3: Probable ABC transporter permease protein NosY





• Molecule 3: Probable ABC transporter permease protein NosY





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138319	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor



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: 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).

Mal	Mol Chain		Bond lengths		ond angles
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.45	0/3204	0.73	4/4349 (0.1%)
2	В	0.42	0/2402	0.65	$2/3247 \ (0.1\%)$
2	С	0.43	0/2402	0.67	1/3247~(0.0%)
3	D	0.44	0/2060	0.63	1/2809~(0.0%)
3	Е	0.40	0/1939	0.70	3/2646~(0.1%)
All	All	0.43	0/12007	0.68	$11/16298 \; (0.1\%)$

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	В	0	1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	A	35	LEU	CA-CB-CG	8.25	134.28	115.30
1	A	182	ASP	CB-CG-OD1	8.13	125.62	118.30
3	Е	112	LEU	CA-CB-CG	6.80	130.94	115.30
3	D	129	LEU	CA-CB-CG	6.49	130.23	115.30
2	В	305	GLU	CA-CB-CG	6.10	126.83	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	В	304	GLN	Peptide

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	3140	0	3017	59	0
2	В	2367	0	2417	21	0
2	С	2367	0	2417	23	0
3	D	2015	0	2136	17	0
3	Е	1896	0	2026	7	0
4	A	1	0	0	0	0
5	A	1	0	0	1	0
All	All	11787	0	12013	116	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 5.

The worst 5 of 116 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:301:ASN:H	1:A:324:ASN:HD22	1.37	0.71
1:A:118:ALA:H	1:A:140:VAL:HG12	1.64	0.63
1:A:141:GLN:HG2	1:A:171:ARG:HB3	1.82	0.61
1:A:116:GLU:HG2	1:A:117:ARG:HG3	1.83	0.59
2:C:224:ARG:HB2	2:C:283:HIS:HB2	1.83	0.59

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	Perce	ntiles
1	A	400/436~(92%)	367 (92%)	33 (8%)	0	100	100
2	В	305/308~(99%)	281 (92%)	24 (8%)	0	100	100
2	С	305/308~(99%)	271 (89%)	33 (11%)	1 (0%)	41	41
3	D	263/276~(95%)	258 (98%)	5 (2%)	0	100	100
3	E	242/276 (88%)	234 (97%)	8 (3%)	0	100	100
All	All	1515/1604 (94%)	1411 (93%)	103 (7%)	1 (0%)	54	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	С	277	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 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	339/365~(93%)	336 (99%)	3 (1%)	78 78
2	В	$250/251\ (100\%)$	250 (100%)	0	100 100
2	С	$250/251 \; (100\%)$	250 (100%)	0	100 100
3	D	205/212 (97%)	204 (100%)	1 (0%)	88 88
3	E	193/212 (91%)	191 (99%)	2 (1%)	76 76
All	All	1237/1291 (96%)	1231 (100%)	6 (0%)	89 88

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	183	PHE
3	Е	112	LEU
3	Е	183	PHE
1	A	279	MET

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Mol	Chain	Res	Type
1	A	132	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	417	HIS
2	С	245	HIS
2	В	261	ASN
2	С	283	HIS
1	A	179	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12690. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal surface views (i)

This section was not generated.

6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section was not generated.

