



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:23 PM UTC

PDB ID : 7NDF / pdb_00007ndf
Title : Crystal structure of nanobody Nb_MsbA#1 in complex with the nucleotide binding domain of MsbA
Authors : Meier, G.; Seeger, M.
Deposited on : 2021-02-01
Resolution : 2.10 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

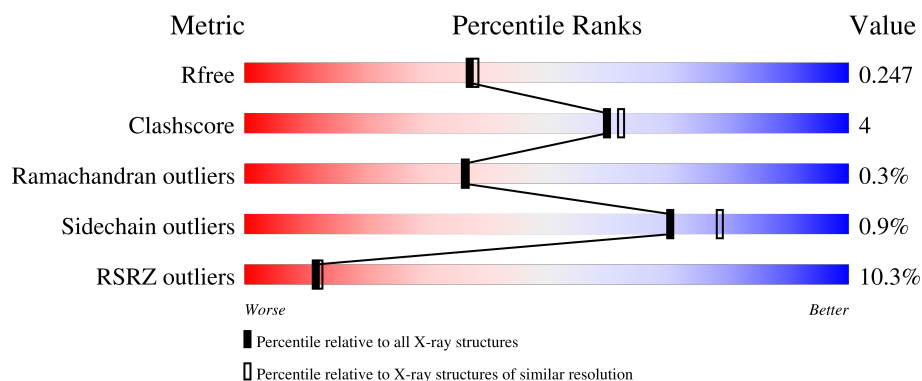
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	C	116	2% 91% 6% ••
1	D	116	9% 91% 6% •
2	A	245	12% 87% 11% ••
2	B	245	13% 84% 13% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5712 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 Nb_MsbA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	113	Total	C	N	O	S	0	0	0
			849	529	149	167	4			
1	D	113	Total	C	N	O	S	0	0	0
			849	529	149	167	4			

- Molecule 2 is a protein called Lipid A ABC transporter ATP-binding protein/permease MsbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	241	Total	C	N	O	S	0	0	0
			1880	1167	340	368	5			
2	B	240	Total	C	N	O	S	0	0	0
			1869	1158	339	367	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	SER	-	expression tag	UNP A0A786F4A3
A	583	ALA	-	expression tag	UNP A0A786F4A3
B	339	SER	-	expression tag	UNP A0A786F4A3
B	583	ALA	-	expression tag	UNP A0A786F4A3

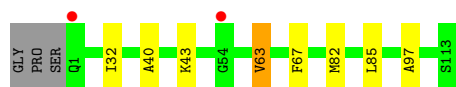
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	48	Total	O	0	0
			48	48		
3	D	27	Total	O	0	0
			27	27		
3	A	86	Total	O	0	0
			86	86		
3	B	104	Total	O	0	0
			104	104		

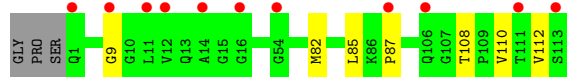
3 Residue-property plots [i](#)

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 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 ($RSRZ > 2$). 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.

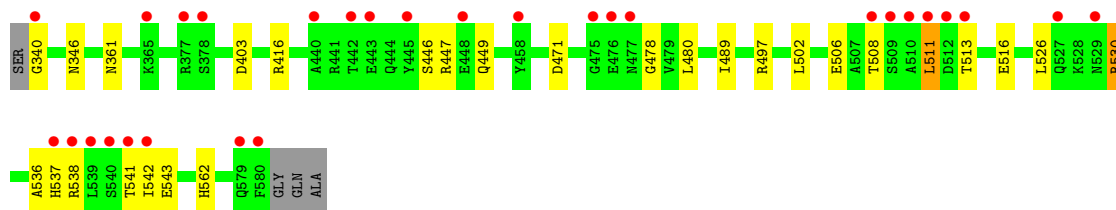
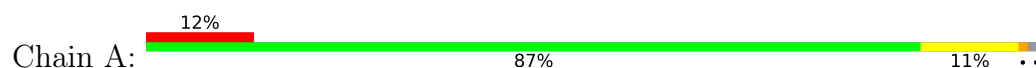
- Molecule 1: Nb_MsbA 1



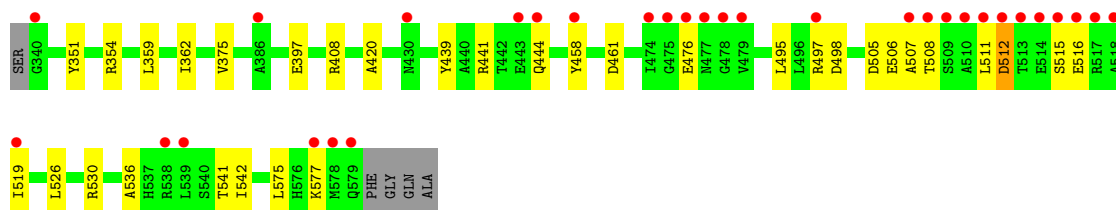
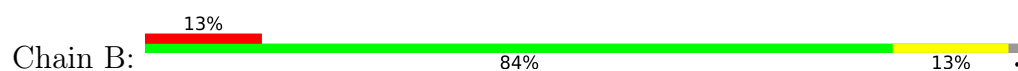
- Molecule 1: Nb_MsbA 1



- Molecule 2: Lipid A ABC transporter ATP-binding protein/permease MsbA



- Molecule 2: Lipid A ABC transporter ATP-binding protein/permease MsbA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.53Å 99.30Å 142.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.41 – 2.10 47.41 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.41-2.10) 100.0 (47.41-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.205 , 0.244 0.209 , 0.247	Depositor DCC
R_{free} test set	2670 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5712	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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	C	0.25	0/865	0.48	0/1170
1	D	0.18	0/865	0.36	0/1170
2	A	0.23	0/1902	0.43	0/2572
2	B	0.27	0/1890	0.44	0/2556
All	All	0.24	0/5522	0.43	0/7468

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	C	849	0	839	6	0
1	D	849	0	839	3	0
2	A	1880	0	1880	18	0
2	B	1869	0	1871	23	0
3	A	86	0	0	0	0
3	B	104	0	0	3	0
3	C	48	0	0	0	0
3	D	27	0	0	0	0
All	All	5712	0	5429	47	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 4.

All (47) 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)
2:B:498:ASP:OD1	2:B:530:ARG:NH2	2.19	0.76
1:C:40:ALA:H	1:C:43:LYS:HE2	1.56	0.69
2:B:511:LEU:HG	2:B:516:GLU:HB3	1.80	0.64
1:C:63:VAL:HG13	1:C:67:PHE:HB2	1.78	0.63
2:A:513:THR:H	2:A:516:GLU:HB3	1.65	0.60
1:C:82:MET:HE2	1:C:85:LEU:HD21	1.84	0.60
2:B:420:ALA:HA	2:B:497:ARG:HH12	1.65	0.60
2:A:447:ARG:NH2	2:A:471:ASP:OD1	2.36	0.58
2:B:359:LEU:HB3	2:B:362:ILE:HD13	1.87	0.57
2:A:502:LEU:HB2	2:A:530:ARG:HD3	1.88	0.56
2:A:480:LEU:HD21	2:B:507:ALA:HB1	1.87	0.56
2:A:526:LEU:O	2:A:530:ARG:HD2	2.06	0.55
2:A:416:ARG:O	2:A:497:ARG:NH1	2.39	0.55
1:D:82:MET:HE2	1:D:85:LEU:HD21	1.90	0.53
2:B:351:TYR:HB2	2:B:354:ARG:HG3	1.91	0.53
1:C:32:ILE:HD12	1:C:97:ALA:HB1	1.92	0.52
2:B:375:VAL:HG12	2:B:536:ALA:HB3	1.91	0.52
2:A:511:LEU:HG	2:A:516:GLU:HB2	1.92	0.52
2:B:526:LEU:O	2:B:530:ARG:NH1	2.42	0.51
2:A:536:ALA:HB3	2:A:542:ILE:HD11	1.93	0.51
2:A:506:GLU:OE2	2:A:541:THR:OG1	2.23	0.51
2:A:537:HIS:NE2	2:B:476:GLU:HB3	2.24	0.51
1:D:87:PRO:HA	1:D:112:VAL:HB	1.95	0.49
2:B:458:TYR:HB2	2:B:519:ILE:HD11	1.95	0.48
2:B:505:ASP:O	2:B:507:ALA:N	2.46	0.47
2:B:575:LEU:C	2:B:577:LYS:H	2.22	0.47
2:B:512:ASP:OD1	2:B:512:ASP:N	2.47	0.46
1:C:40:ALA:N	1:C:43:LYS:HE2	2.28	0.46
2:B:408:ARG:NH1	3:B:607:HOH:O	2.47	0.46
2:B:516:GLU:N	2:B:516:GLU:OE1	2.49	0.46
2:B:515:SER:O	2:B:519:ILE:HG12	2.16	0.46
2:B:461:ASP:HB3	3:B:632:HOH:O	2.16	0.45
2:A:508:THR:OG1	2:A:538:ARG:NH1	2.47	0.45
1:D:9:GLY:HA3	1:D:108:THR:HG22	1.98	0.44
2:A:543:GLU:HG2	2:A:562:HIS:CE1	2.53	0.44
2:A:542:ILE:HD13	2:A:542:ILE:HA	1.65	0.43
2:B:441:ARG:HE	2:B:444:GLN:CD	2.27	0.43
2:B:439:TYR:HD2	2:B:497:ARG:NE	2.17	0.42
2:A:446:SER:HB3	2:A:449:GLN:HG3	2.01	0.42
2:B:536:ALA:HB2	2:B:542:ILE:HG21	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:340:GLY:HA2	2:A:403:ASP:OD1	2.20	0.42
2:B:495:LEU:HD23	2:B:526:LEU:HD13	2.02	0.42
2:A:346:ASN:OD1	2:A:361:ASN:ND2	2.51	0.41
2:A:489:ILE:HD13	2:A:489:ILE:HA	1.89	0.41
1:C:40:ALA:HB3	1:C:43:LYS:HG2	2.03	0.41
2:A:478:GLY:HA2	2:B:508:THR:HA	2.04	0.40
2:B:397:GLU:OE2	3:B:601:HOH:O	2.21	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	C	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
1	D	111/116 (96%)	109 (98%)	2 (2%)	0	100	100
2	A	239/245 (98%)	231 (97%)	8 (3%)	0	100	100
2	B	238/245 (97%)	231 (97%)	5 (2%)	2 (1%)	16	12
All	All	699/722 (97%)	679 (97%)	18 (3%)	2 (0%)	36	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	506	GLU
2	B	512	ASP

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	C	90/92 (98%)	89 (99%)	1 (1%)	65	74
1	D	90/92 (98%)	89 (99%)	1 (1%)	65	74
2	A	201/203 (99%)	199 (99%)	2 (1%)	68	76
2	B	200/203 (98%)	199 (100%)	1 (0%)	81	88
All	All	581/590 (98%)	576 (99%)	5 (1%)	70	78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	63	VAL
1	D	110	VAL
2	A	511	LEU
2	A	530	ARG
2	B	541	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	579	GLN
2	B	346	ASN
2	B	361	ASN
2	B	576	HIS

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

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.

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	C	113/116 (97%)	0.14	2 (1%) 67 70	28, 43, 71, 79	0
1	D	113/116 (97%)	0.71	11 (9%) 13 14	38, 63, 93, 103	0
2	A	241/245 (98%)	0.46	29 (12%) 9 9	28, 44, 83, 114	0
2	B	240/245 (97%)	0.52	31 (12%) 7 8	27, 40, 108, 133	0
All	All	707/722 (97%)	0.47	73 (10%) 12 12	27, 46, 88, 133	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	539	LEU	6.9
2	B	508	THR	6.6
2	A	511	LEU	6.5
2	A	580	PHE	6.3
2	B	510	ALA	6.2
2	B	511	LEU	5.8
2	B	509	SER	5.0
2	B	477	ASN	4.8
2	A	542	ILE	4.7
2	B	476	GLU	4.6
2	A	510	ALA	4.3
2	B	475	GLY	4.3
2	A	540	SER	4.3
2	B	340	GLY	4.2
2	A	508	THR	4.1
2	A	440	ALA	4.1
2	B	579	GLN	4.1
2	A	513	THR	4.0
2	B	578	MET	3.9
2	A	538	ARG	3.8
2	B	515	SER	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	513	THR	3.7
2	A	377	ARG	3.7
2	A	541	THR	3.7
2	B	516	GLU	3.6
2	B	507	ALA	3.5
2	B	517	ARG	3.5
2	B	479	VAL	3.5
2	B	478	GLY	3.4
2	A	509	SER	3.2
2	B	458	TYR	3.1
2	A	340	GLY	3.1
2	B	539	LEU	3.0
1	D	16	GLY	3.0
2	A	443	GLU	2.9
2	B	577	LYS	2.9
2	A	445	TYR	2.8
2	A	537	HIS	2.8
2	B	514	GLU	2.8
2	B	474	ILE	2.7
1	D	11	LEU	2.6
2	A	512	ASP	2.6
1	D	14	ALA	2.6
2	B	518	ALA	2.6
2	A	442	THR	2.6
2	A	476	GLU	2.6
2	B	519	ILE	2.6
1	D	54	GLY	2.5
2	B	386	ALA	2.5
2	B	497	ARG	2.4
1	D	9	GLY	2.4
2	A	477	ASN	2.4
2	A	475	GLY	2.4
1	D	113	SER	2.4
2	A	365	LYS	2.4
2	A	529	ASN	2.3
1	D	111	THR	2.2
2	B	512	ASP	2.2
2	A	448	GLU	2.2
2	B	538	ARG	2.2
2	B	443	GLU	2.1
1	D	1	GLN	2.1
1	D	12	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	106	GLN	2.1
2	A	527	GLN	2.1
1	C	54	GLY	2.1
2	B	430	ASN	2.1
1	C	1	GLN	2.1
2	A	378	SER	2.1
2	B	444	GLN	2.0
2	A	579	GLN	2.0
1	D	87	PRO	2.0
2	A	458	TYR	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 oligosaccharides 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.