

Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 10:01 AM EDT

PDB ID	:	4N8M
Title	:	Structural polymorphism in the N-terminal oligomerization domain of NPM1
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Deposited on	:	2013-10-17
Resolution	:	1.80 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 (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:

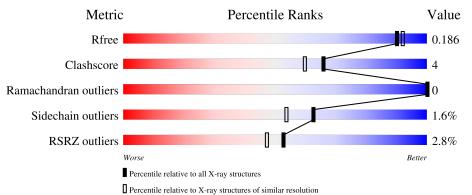
Refmac CCP4	: : : :	 1.13 2.35.1 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (proteins) Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.80 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793(1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	А	133	75%	6%	19%			
1	В	133	73%	8%	20%			
1	С	133	73%	7%	20%			
1	D	133	^{2%} 71%	8%	21%			
1	Е	133	^{2%} 70%	10%	20%			



4N8M

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4263 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	108	Total	С	Ν	0	S	0	3	0
	A	108	824	521	139	159	5	0	J	0
1	В	107	Total	С	Ν	Ο	S	0	1	0
1	D	107	810	513	138	155	4	0		0
1	1 0	C 106	Total	С	Ν	0	S	0	1	0
	U		802	509	136	153	4			
1	D	105	Total	С	Ν	0	S	0	0	0
	D	105	787	501	135	147	4	0		0
1	Е	106	Total	С	Ν	Ο	S	0	2	0
	Ľ	100	808	512	137	155	4	0	Δ	0

• Molecule 1 is a protein called Nucleophosmin.

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-2	GLY	-	expression tag	UNP Q61937
А	-1	SER	-	expression tag	UNP Q61937
А	0	HIS	-	expression tag	UNP Q61937
В	-2	GLY	-	expression tag	UNP Q61937
В	-1	SER	-	expression tag	UNP Q61937
В	0	HIS	-	expression tag	UNP Q61937
С	-2	GLY	-	expression tag	UNP Q61937
С	-1	SER	-	expression tag	UNP Q61937
С	0	HIS	-	expression tag	UNP Q61937
D	-2	GLY	-	expression tag	UNP Q61937
D	-1	SER	-	expression tag	UNP Q61937
D	0	HIS	-	expression tag	UNP Q61937
Е	-2	GLY	-	expression tag	UNP Q61937
Е	-1	SER	-	expression tag	UNP Q61937
Е	0	HIS	_	expression tag	UNP Q61937

• Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Co 1 1	0	0
2	В	1	Total Co 1 1	0	0
2	С	1	Total Co 1 1	0	0
2	D	1	Total Co 1 1	0	0
2	Е	1	Total Co 1 1	0	0

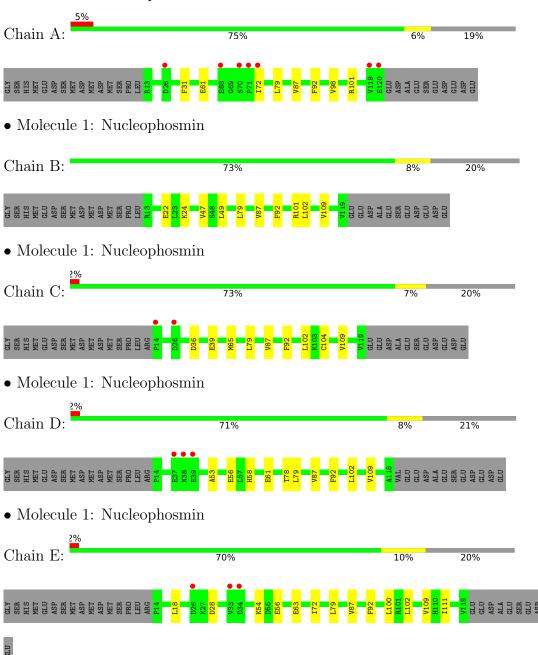
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	42	$\begin{array}{cc} \text{Total} & \text{O} \\ 42 & 42 \end{array}$	0	0
3	В	58	$\begin{array}{cc} \text{Total} & \text{O} \\ 58 & 58 \end{array}$	0	0
3	С	48	Total O 48 48	0	0
3	D	40	Total O 40 40	0	0
3	Ε	39	Total O 39 39	0	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 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: Nucleophosmin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	90.67Å 69.79Å 88.63Å	Depositor
a, b, c, α , β , γ	90.00° 99.87° 90.00°	Depositor
Resolution (Å)	37.26 - 1.80	Depositor
	44.47 - 1.80	EDS
% Data completeness	97.2 (37.26-1.80)	Depositor
(in resolution range)	$97.2 \ (44.47 - 1.80)$	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	3.12 (at 1.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
B B.	0.163 , 0.190	Depositor
R, R_{free}	0.158 , 0.186	DCC
R_{free} test set	2493 reflections $(5.09%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	20.1	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38 , 52.3	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4263	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.99% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: CO

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	Bo	nd lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.39	0/849	0.61	0/1151	
1	В	0.45	0/829	0.66	0/1124	
1	С	0.48	1/821~(0.1%)	0.60	0/1113	
1	D	0.39	0/803	0.62	1/1088~(0.1%)	
1	Ε	0.36	0/830	0.57	0/1124	
All	All	0.42	1/4132~(0.0%)	0.61	1/5600~(0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	С	104	CYS	CB-SG	-6.57	1.71	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	53	ALA	N-CA-C	-5.20	96.95	111.00

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	А	824	0	818	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	810	0	804	7	0
1	С	802	0	799	6	0
1	D	787	0	786	6	0
1	Ε	808	0	808	8	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	Ε	1	0	0	0	0
3	А	42	0	0	0	0
3	В	58	0	0	0	0
3	С	48	0	0	1	0
3	D	40	0	0	0	0
3	Е	39	0	0	0	0
All	All	4263	0	4015	32	0

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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 (32) close contacts	within the same	ne asymmetric	e unit are	e listed belo	w, sorted by	their clash
magnitude.						

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:C:79:LEU:HD21	1:C:87:VAL:HG23	1.59	0.85
1:C:36:ASP:HB3	1:C:39:GLU:HG2	1.67	0.76
1:D:79:LEU:HD21	1:D:87:VAL:HG23	1.67	0.74
1:C:79:LEU:CD2	1:C:87:VAL:HG23	2.17	0.73
1:B:79:LEU:CD2	1:B:87:VAL:HG23	2.24	0.67
1:A:79:LEU:CD2	1:A:87:VAL:HG23	2.28	0.64
1:C:79:LEU:HD21	1:C:87:VAL:CG2	2.28	0.63
1:E:102:LEU:HD21	1:E:109:VAL:HG21	1.80	0.62
1:B:102:LEU:HD21	1:B:109:VAL:HG21	1.79	0.62
1:D:79:LEU:HD21	1:D:87:VAL:CG2	2.29	0.61
1:A:31:PHE:HB3	1:A:98:VAL:HG13	1.82	0.61
1:E:79:LEU:CD2	1:E:87:VAL:HG23	2.31	0.60
1:D:79:LEU:CD2	1:D:87:VAL:HG23	2.33	0.59
1:B:79:LEU:HD23	1:B:87:VAL:HG23	1.86	0.56
1:A:79:LEU:HD21	1:A:87:VAL:HG23	1.89	0.53
1:C:102:LEU:HD21	1:C:109:VAL:HG21	1.89	0.52
1:E:28:ASP:HB2	1:E:100:LEU:O	2.11	0.51
1:A:61:GLU:OE1	1:A:101:ARG:HD2	2.12	0.50
1:E:54:LYS:HB2	1:E:56:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:HD11	1:E:18:LEU:O	2.13	0.49
1:D:102:LEU:HD21	1:D:109:VAL:HG21	1.96	0.48
1:E:100:LEU:HD13	1:E:111:ILE:HD12	1.97	0.46
1:B:49:LEU:HD23	1:B:109:VAL:HG22	2.00	0.43
1:E:63:GLU:HA	1:E:72:ILE:O	2.18	0.43
1:E:79:LEU:HD21	1:E:87:VAL:HG23	1.98	0.43
1:B:47:VAL:HG12	1:B:79:LEU:HD11	2.02	0.42
1:D:56:GLU:HG3	1:D:58:HIS:CE1	2.55	0.41
1:D:78:THR:O	1:D:79:LEU:HD23	2.20	0.41
1:C:65:MET:HG2	3:C:309:HOH:O	2.20	0.41
1:A:79:LEU:HD23	1:A:87:VAL:HG23	2.01	0.41
1:B:79:LEU:HD21	1:B:87:VAL:HG23	2.02	0.40
1:B:22:GLU:OE2	1:B:24:LYS:HE3	2.21	0.40

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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	А	109/133~(82%)	104 (95%)	5 (5%)	0	100 100
1	В	106/133~(80%)	102 (96%)	4 (4%)	0	100 100
1	С	105/133~(79%)	99~(94%)	6~(6%)	0	100 100
1	D	103/133~(77%)	98~(95%)	5 (5%)	0	100 100
1	Ε	106/133~(80%)	103 (97%)	3(3%)	0	100 100
All	All	529/665~(80%)	506 (96%)	23~(4%)	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	92/115~(80%)	91~(99%)	1 (1%)	73 68
1	В	89/115~(77%)	87~(98%)	2(2%)	52 39
1	С	88/115 (76%)	87~(99%)	1 (1%)	73 68
1	D	85/115 (74%)	83~(98%)	2(2%)	49 36
1	Е	90/115~(78%)	89~(99%)	1 (1%)	73 68
All	All	444/575~(77%)	437~(98%)	7~(2%)	62 54

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	92	PHE
1	В	92	PHE
1	В	101	ARG
1	С	92	PHE
1	D	61	GLU
1	D	92	PHE
1	Е	92	PHE

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

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 5 ligands modelled in this entry, 5 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 (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, 95^{th} 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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(A^2)$	$\mathbf{Q}{<}0.9$
1	А	108/133~(81%)	-0.01	7 (6%) 18 15	12, 24, 54, 71	0
1	В	107/133~(80%)	-0.16	0 100 100	10, 20, 47, 57	0
1	С	106/133~(79%)	-0.27	2 (1%) 66 63	13, 22, 52, 78	0
1	D	105/133~(78%)	-0.16	3 (2%) 51 46	15, 26, 65, 95	0
1	Ε	106/133~(79%)	-0.20	3 (2%) 53 47	17, 30, 60, 73	0
All	All	532/665~(80%)	-0.16	15 (2%) 53 47	10, 24, 56, 95	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	37	GLU	5.8
1	Е	33	VAL	4.6
1	Е	26	ASP	3.8
1	А	119	VAL	3.4
1	А	68	GLU	3.0
1	С	14	PRO	2.9
1	А	120	GLU	2.8
1	D	38	ASN	2.8
1	С	26	ASP	2.7
1	А	70	SER	2.6
1	Ε	34	ASP	2.6
1	А	26	ASP	2.5
1	А	71	PRO	2.3
1	А	72	ILE	2.1
1	D	39	GLU	2.1

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 monosaccharides 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, 95^{th} 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	CO	А	601	1/1	0.87	0.16	76,76,76,76	0
2	CO	Е	201	1/1	0.91	0.19	85,85,85,85	0
2	CO	D	201	1/1	0.94	0.04	64,64,64,64	0
2	CO	С	201	1/1	0.94	0.13	58, 58, 58, 58	0
2	CO	В	201	1/1	0.96	0.04	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.

