



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:14 AM EDT

PDB ID : 6DFD / pdb\_00006dfd  
Title : Crystal structure of CNNM3 cyclic nucleotide-binding homology domain  
Authors : Kozlov, G.; Gehring, K.  
Deposited on : 2018-05-14  
Resolution : 1.90 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](mailto: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>.

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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

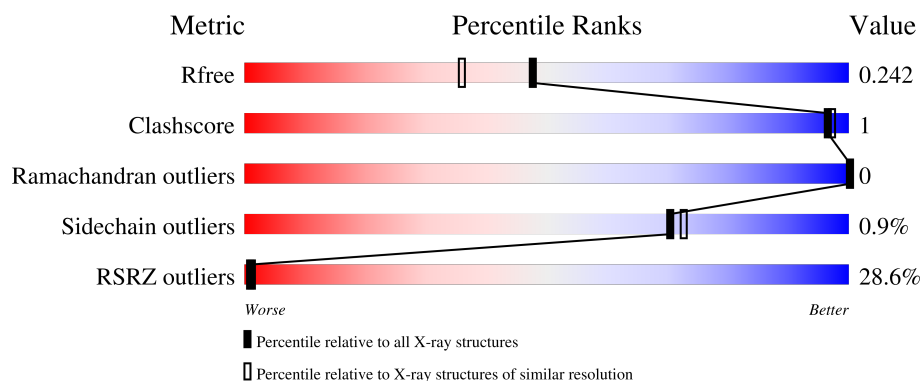
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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  $\geq 3$ , 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	260	<div> <div>5%</div> <div>51%</div> <div>47%</div> </div>
1	B	260	<div> <div>23%</div> <div>47%</div> <div>52%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4240 atoms, of which 2097 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 Metal transporter CNNM3.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	137	Total	C	H	N	O	S	Se	0	0	0
			2251	721	1135	190	200	1	4			
1	B	125	Total	C	H	N	O	S	Se	0	0	0
			1919	621	962	163	169	1	3			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	448	GLY	-	expression tag	UNP Q8NE01
A	449	PRO	-	expression tag	UNP Q8NE01
A	450	LEU	-	expression tag	UNP Q8NE01
A	451	GLY	-	expression tag	UNP Q8NE01
A	452	SER	-	expression tag	UNP Q8NE01
A	516	MSE	ILE	engineered mutation	UNP Q8NE01
A	591	MSE	THR	engineered mutation	UNP Q8NE01
A	623	MSE	ALA	engineered mutation	UNP Q8NE01
A	651	MSE	LEU	engineered mutation	UNP Q8NE01
A	669	MSE	VAL	engineered mutation	UNP Q8NE01
A	670	MSE	ILE	engineered mutation	UNP Q8NE01
B	448	GLY	-	expression tag	UNP Q8NE01
B	449	PRO	-	expression tag	UNP Q8NE01
B	450	LEU	-	expression tag	UNP Q8NE01
B	451	GLY	-	expression tag	UNP Q8NE01
B	452	SER	-	expression tag	UNP Q8NE01
B	516	MSE	ILE	engineered mutation	UNP Q8NE01
B	591	MSE	THR	engineered mutation	UNP Q8NE01
B	623	MSE	ALA	engineered mutation	UNP Q8NE01
B	651	MSE	LEU	engineered mutation	UNP Q8NE01
B	669	MSE	VAL	engineered mutation	UNP Q8NE01
B	670	MSE	ILE	engineered mutation	UNP Q8NE01

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	64	Total 64	O 64	0	0
2	B	6	Total 6	O 6	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.27Å 101.27Å 77.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.47 – 1.90 32.47 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (32.47-1.90) 99.6 (32.47-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 1.91Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.219 , 0.239 0.222 , 0.242	Depositor DCC
$R_{free}$ test set	1591 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4240	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	A	0.25	0/1135	0.46	0/1530
1	B	0.15	0/971	0.36	0/1314
All	All	0.21	0/2106	0.42	0/2844

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	A	1116	1135	1133	2	0
1	B	957	962	927	2	0
2	A	64	0	0	1	1
2	B	6	0	0	0	0
All	All	2143	2097	2060	4	1

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 1.

All (4) 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:B:565:ARG:NH1	1:B:578:GLU:OE2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:LYS:NZ	2:A:801:HOH:O	2.31	0.61
1:A:569:GLU:HA	1:A:575:LEU:O	2.17	0.44
1:B:650:LEU:O	1:B:652:ALA:N	2.54	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:854:HOH:O	2:A:854:HOH:O[7_555]	1.57	0.63

## 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	133/260 (51%)	128 (96%)	5 (4%)	0	100	100
1	B	121/260 (46%)	119 (98%)	2 (2%)	0	100	100
All	All	254/520 (49%)	247 (97%)	7 (3%)	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	123/225 (55%)	121 (98%)	2 (2%)	55	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	95/225 (42%)	95 (100%)	0	100	100
All	All	218/450 (48%)	216 (99%)	2 (1%)	70	73

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

Mol	Chain	Res	Type
1	A	562	LEU
1	A	569	GLU

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	133/260 (51%)	0.63	13 (9%) 13 13	33, 49, 84, 106	0
1	B	122/260 (46%)	2.08	60 (49%) 0 0	49, 82, 121, 142	0
All	All	255/520 (49%)	1.32	73 (28%) 1 1	33, 64, 115, 142	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	LEU	6.7
1	A	653	THR	6.6
1	B	499	ALA	6.3
1	B	624	TYR	6.1
1	B	521	LEU	5.2
1	B	520	VAL	5.1
1	B	497	LEU	5.1
1	B	650	LEU	4.8
1	B	517	SER	4.2
1	B	529	SER	4.1
1	A	488	TYR	4.0
1	B	540	ASN	4.0
1	B	555	VAL	3.9
1	B	518	GLU	3.9
1	B	523	HIS	3.8
1	B	506	ARG	3.7
1	B	547	TYR	3.6
1	A	553	GLN	3.6
1	B	527	HIS	3.6
1	B	522	LEU	3.6
1	A	624	TYR	3.5
1	B	652	ALA	3.5
1	A	490	VAL	3.4
1	B	637	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	515	ARG	3.3
1	B	539	SER	3.3
1	A	655	ALA	3.2
1	B	500	THR	3.1
1	B	544	THR	3.0
1	B	577	PHE	3.0
1	B	528	PRO	2.9
1	B	509	ASP	2.9
1	B	501	GLN	2.8
1	B	505	SER	2.8
1	A	652	ALA	2.8
1	B	530	VAL	2.8
1	A	648	ASN	2.7
1	B	554	PRO	2.7
1	B	649	ALA	2.7
1	A	625	CYS	2.7
1	B	537	ASP	2.6
1	B	507	GLU	2.6
1	B	629	THR	2.6
1	B	643	ARG	2.5
1	B	543	ALA	2.5
1	A	552	SER	2.5
1	B	508	VAL	2.5
1	B	512	SER	2.4
1	B	519	LYS	2.4
1	B	513	PRO	2.4
1	B	550	GLN	2.4
1	B	562	LEU	2.3
1	B	561	ILE	2.3
1	A	551	ARG	2.3
1	B	648	ASN	2.3
1	B	525	LEU	2.2
1	B	575	LEU	2.2
1	B	552	SER	2.2
1	B	556	ASP	2.2
1	B	574	GLY	2.1
1	B	647	LEU	2.1
1	A	519	LYS	2.1
1	B	498	LEU	2.1
1	B	542	LEU	2.1
1	B	553	GLN	2.1
1	B	582	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	635	ASP	2.1
1	B	587	VAL	2.1
1	B	638	LEU	2.1
1	B	589	ALA	2.1
1	A	572	LYS	2.0
1	B	503	PHE	2.0
1	B	502	ARG	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.