



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 09:29 PM UTC

PDB ID : 4LOG / pdb\_00004log  
Title : The crystal structure of the orphan nuclear receptor PNR ligand binding domain fused with MBP  
Authors : Tan, M.E.; Zhou, X.E.; Soon, F.-F.; Li, X.; Li, J.; Yong, E.-L.; Melcher, K.; Xu, H.E.  
Deposited on : 2013-07-12  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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>.

---

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

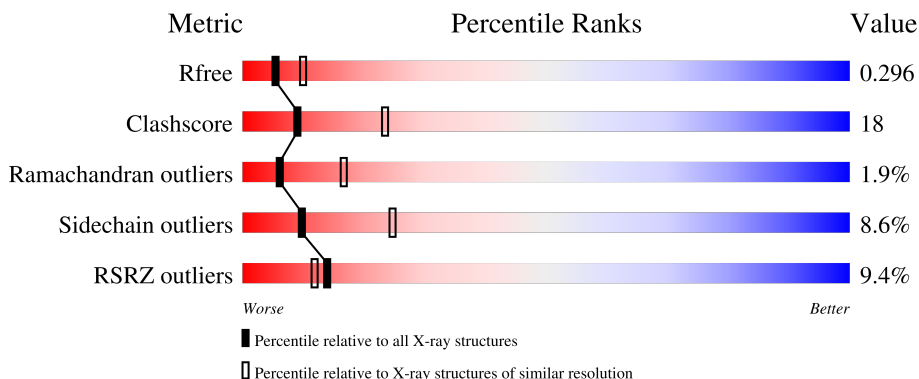
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	574	
1	B	574	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 6234 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 Maltose ABC transporter periplasmic protein and NR2E3 protein chimeric construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	553	4334	2799	712	809	14	0	0	0
1	B	232	1838	1184	314	330	10	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP K0BGG6
A	369	ASN	-	linker	UNP K0BGG6
A	370	ALA	-	linker	UNP K0BGG6
A	371	ALA	-	linker	UNP K0BGG6
A	372	ALA	-	linker	UNP K0BGG6
A	1215	GLU	-	linker	UNP K0BGG6
A	1216	PHE	-	linker	UNP K0BGG6
A	1405	SER	CYS	engineered mutation	UNP Q8IVZ9
A	1411	HIS	-	expression tag	UNP Q8IVZ9
A	1412	HIS	-	expression tag	UNP Q8IVZ9
A	1413	HIS	-	expression tag	UNP Q8IVZ9
A	1414	HIS	-	expression tag	UNP Q8IVZ9
A	1415	HIS	-	expression tag	UNP Q8IVZ9
A	1416	HIS	-	expression tag	UNP Q8IVZ9
B	1	MET	-	initiating methionine	UNP K0BGG6
B	369	ASN	-	linker	UNP K0BGG6
B	370	ALA	-	linker	UNP K0BGG6
B	371	ALA	-	linker	UNP K0BGG6
B	372	ALA	-	linker	UNP K0BGG6
B	1215	GLU	-	linker	UNP K0BGG6
B	1216	PHE	-	linker	UNP K0BGG6
B	1405	SER	CYS	engineered mutation	UNP Q8IVZ9
B	1411	HIS	-	expression tag	UNP Q8IVZ9
B	1412	HIS	-	expression tag	UNP Q8IVZ9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	1413	HIS	-	expression tag	UNP Q8IVZ9
B	1414	HIS	-	expression tag	UNP Q8IVZ9
B	1415	HIS	-	expression tag	UNP Q8IVZ9
B	1416	HIS	-	expression tag	UNP Q8IVZ9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	33	Total O 33 33	0	0
2	B	29	Total O 29 29	0	0





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.44Å 184.94Å 85.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-2.70) 96.5 (30.00-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.68Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.285 , 0.307 0.278 , 0.296	Depositor DCC
$R_{free}$ test set	2961 reflections (7.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.2	Xtrriage
Anisotropy	0.176	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 33.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.017 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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	0.74	0/4439	0.84	0/6025
1	B	0.85	0/1879	0.95	3/2548 (0.1%)
All	All	0.78	0/6318	0.87	3/8573 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1280	PRO	N-CA-C	10.00	122.90	110.70
1	B	1279	ALA	CA-C-N	-7.82	112.33	120.38
1	B	1279	ALA	C-N-CA	-7.82	112.33	120.38

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	4334	0	4340	168	0
1	B	1838	0	1875	74	0
2	A	33	0	0	6	0
2	B	29	0	0	2	0
All	All	6234	0	6215	228	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 18.

The worst 5 of 228 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:1302:VAL:O	1:B:1306:THR:HG22	1.50	1.12
1:A:61:ILE:HD11	1:A:266:ALA:HB1	1.46	0.96
1:A:1275:CYS:HB2	1:A:1276:PRO:HD3	1.68	0.76
1:A:152:ASN:HD21	1:A:155:GLU:HG2	1.53	0.74
1:A:9:LEU:HD21	1:A:37:VAL:HG22	1.69	0.73

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	549/574 (96%)	488 (89%)	53 (10%)	8 (2%)	8 22
1	B	228/574 (40%)	199 (87%)	22 (10%)	7 (3%)	3 8
All	All	777/1148 (68%)	687 (88%)	75 (10%)	15 (2%)	6 17

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1276	PRO
1	B	362	ALA
1	B	1281	PRO
1	A	1275	CYS
1	B	1277	LEU

### 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	459/472 (97%)	426 (93%)	33 (7%)	13	32
1	B	201/472 (43%)	177 (88%)	24 (12%)	5	13
All	All	660/944 (70%)	603 (91%)	57 (9%)	10	25

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1366	VAL
1	B	1394	THR
1	B	358	THR
1	B	1393	LYS
1	B	1318	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1356	HIS
1	B	357	GLN
1	B	1364	GLN
1	A	1364	GLN
1	B	1267	GLN

### 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 [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<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	553/574 (96%)	0.54	37 (6%) 24 21	21, 59, 99, 161	0
1	B	232/574 (40%)	0.66	37 (15%) 5 4	21, 50, 112, 148	7 (3%)
All	All	785/1148 (68%)	0.58	74 (9%) 14 12	21, 57, 104, 161	7 (0%)

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	ILE	6.1
1	A	1276	PRO	5.8
1	B	342	TRP	4.8
1	B	1276	PRO	4.8
1	B	1268	TRP	4.8

### 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.